A catalogue of [100], [110], and [111] symmetric tilt boundaries in face-centered cubic hard sphere crystals.

DIVISION OF APPLIED SCIENCES

A CATALOGUE OF
[100], [110], AND [111] SYMMETRIC TILT BOUNDARIES
IN FACE-CENTERED CUBIC HARD SPHERE CRYSTALS

H.J. Frost*, M.F. Ashby**, and F. Spaepen†

Harvard University
Cambridge, Massachusetts

NATIONAL SCIENCE FOUNDATION GRANT DMR 80-20247

MATERIALS RESEARCH LABORATORY

TECHNICAL REPORT

A CATALOGUE OF [100], [110], AND [111] SYMMETRIC TILT BOUNDARIES IN FACE-CENTERED CUBIC HARD SPHERE CRYSTALS

H.J. Frost*, M.F. Ashby**, and F. Spaepen†

*Thayer School of Engineering
Dartmouth College,
Hanover, NH, 03755 USA

**Department of Engineering
University of Cambridge
Cambridge CB2 1PZ, England

†Division of Applied Sciences
Harvard University
Cambridge, MA, 02138, USA

June 1982

The research reported in this document was made possible through support extended the Division of Applied Sciences, Harvard University, by the National Science Foundation under Contract DMR 80-20247.

Division of Applied Sciences
Harvard University, Cambridge, MA 02138

Keywords: grain boundaries, structure, hard spheres, interstitials, substitutionals, density, faceting.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1. INTRODUCTION

This report describes symmetric coincidence tilt-boundaries between f.c.c. crystals made up of hard spheres. The hard-sphere interaction can be thought of as one well-defined limit of the more general soft-sphere interactions used in computer simulations (and certain metals, e.g. aluminum, are made up of ions which interact in an almost hard-sphere way). The hard-sphere solid with minimum energy is that with the maximum density. In constructing such boundaries, it is necessary to have a criterion for choosing among alternative structures with the same tilt axis and angle; we selected the structure which had the maximum density. Three tilt axes and all coincidence densities up to $\Sigma 53$ for [100], $\Sigma 43$ for [110] and $\Sigma 39$ for [111] were examined, 52 boundaries in all.

Having constructed the boundaries, we calculated the coordinates of the centers of the hard spheres, and used these coordinates to calculate

(a) the excess volume of each boundary

(b) the size of all the interstitial sites in the boundary.

(c) the size of all substitutional sites in the boundary.

Finally, we analyzed the structure of each boundary in terms of the packing of polyhedral holes [1-3] and channels. The work is an extension of that published earlier [1,2,4].

2. METHOD

2.1 *Construction of the Boundaries*

The grain boundary models were constructed graphically. Two symmetrical half-crystals were translated with respect to each other until a mechanically stable position which maximized the density without atom overlap was found. This requires at least three contacts across the boundary (i.e. between an atom of one

crystal and atoms of the other) per repeat unit of the boundary. Sometimes the symmetry of the boundary yields a fourth (redundant) contact. With only two contacts between the crystals, per repeat unit, the arrangement can always be densified by a relative displacement of one crystal, which is determined by maintaining the two contacts until a thrid is made.
After fixing the orientations, one crystal has three translational degrees of freedom with respect to the other, and all three must be constrained at the position of minimum density. For more than half the boundaries the densest configuration included a relative displacement in the direction of the tilt axis (the z direction). All [111] boundaries had such a displacement, but only about half the [110] boundaries.

2.2 *Faceting*

Most boundaries are constructed without faceting. We may define faceting by specifying that in a boundary without faceting each half-crystal is composed of all the atoms of that crystal up to a particular crystallographic plane, and none beyond that plane. A faceted boundary has half-crystals which contain some atoms beyond a particular plane (parallel to the boundary) by omitting some atoms that are not beyond that plane. An intermediate case is possible when more than one atom sits in each plane parallel to the boundary (per repeat unit of the boundary), and in which the last plane of the half-crystal retains some atoms and omits others. Our only example of this is [111] Σ21a $(2\bar{3}1)$.

We have concentrated on constructing non-faceted boundaries. We find that faceted boundaries are denser than non-faceted boundaries when a dense plane in one crystal is almost parallel to another dense plane in the other crystal. Good examples are [100] Σ29a, (073) and (052), and [110] Σ41c $(3\bar{3}8)$. If such nearly parallel planes were not obvious, we did not systematically

explore the possibility of faceted arrangements unless no unfaceted boundary could be constructed with excess volume V^{EX} less than 0.5. Several of the [111] tilt boundaries that have a stacking order inversion are shown in faceted arrangements. The excess volume for the faceted arrangements is surprising low compared to the unfaceted ones. It may be possible to construct certain high sigma boundaries in dense faceted arrangements. For example, $\Sigma 85\,(0,11,7)$ appears in a surprisingly dense faceted arrangement. We expect that for boundaries with a tilt axis of lower crystallographic order, the possibility of faceting will become more important.

2.3 *Excess Volume*

All the boundaries have a periodic structure, as discussed in Section 4.1 and illustrated by Fig. 1. A parallelepiped box is constructed with vertices at atom centers well within good crystal, and with two of its faces parallel to the boundary plane and congruent with the boundary repeat unit. If this box has a volume V and contains N atoms, the excess volume associated with one repeat unit of the boundary is $V-N\Omega$, where $\Omega = 0.7071$ is the volume associated with one sphere in the f.c.c. structure (the sphere diameter is unity). It is convenient to express this in units of volume per sphere:

$$V^* = \frac{V-N\Omega}{\Omega}$$

so that V^* becomes the dimensionless excess volume of one repeat unit of the boundary. It is also convenient to express the area of the repeat unit, A, in units of the "area per atom" in the structure $\Omega^{2/3} = 0.7937$:

$$A^* = \frac{A}{\Omega^{2/3}}$$

so that A^* becomes the dimensionless area of one repeat unit of the boundary.

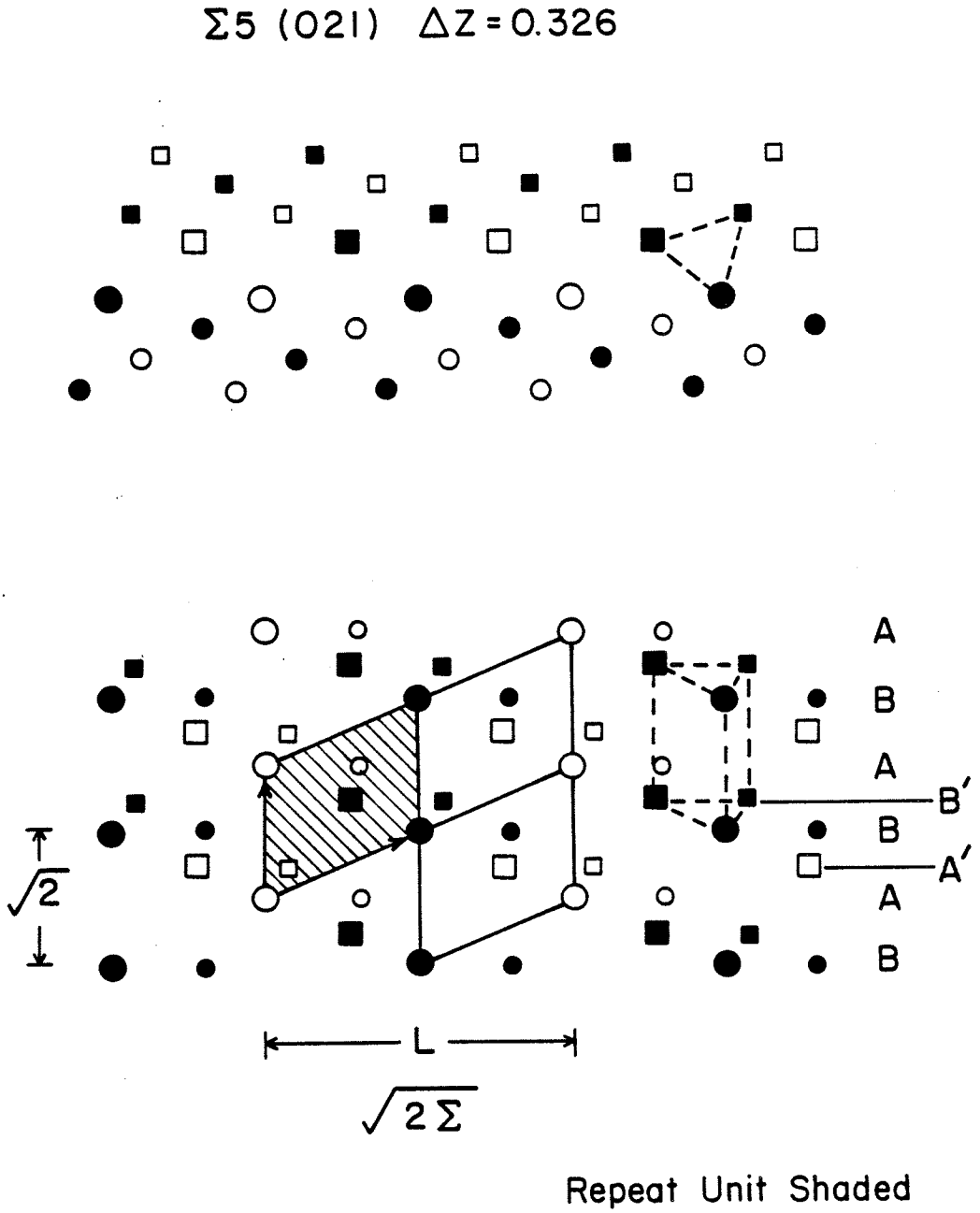


Figure 1(a) Projections of the [100] Σ5 (021) boundary structure onto a plane perpendicular to the tilt axis (top) and onto the boundary plane (bottom).

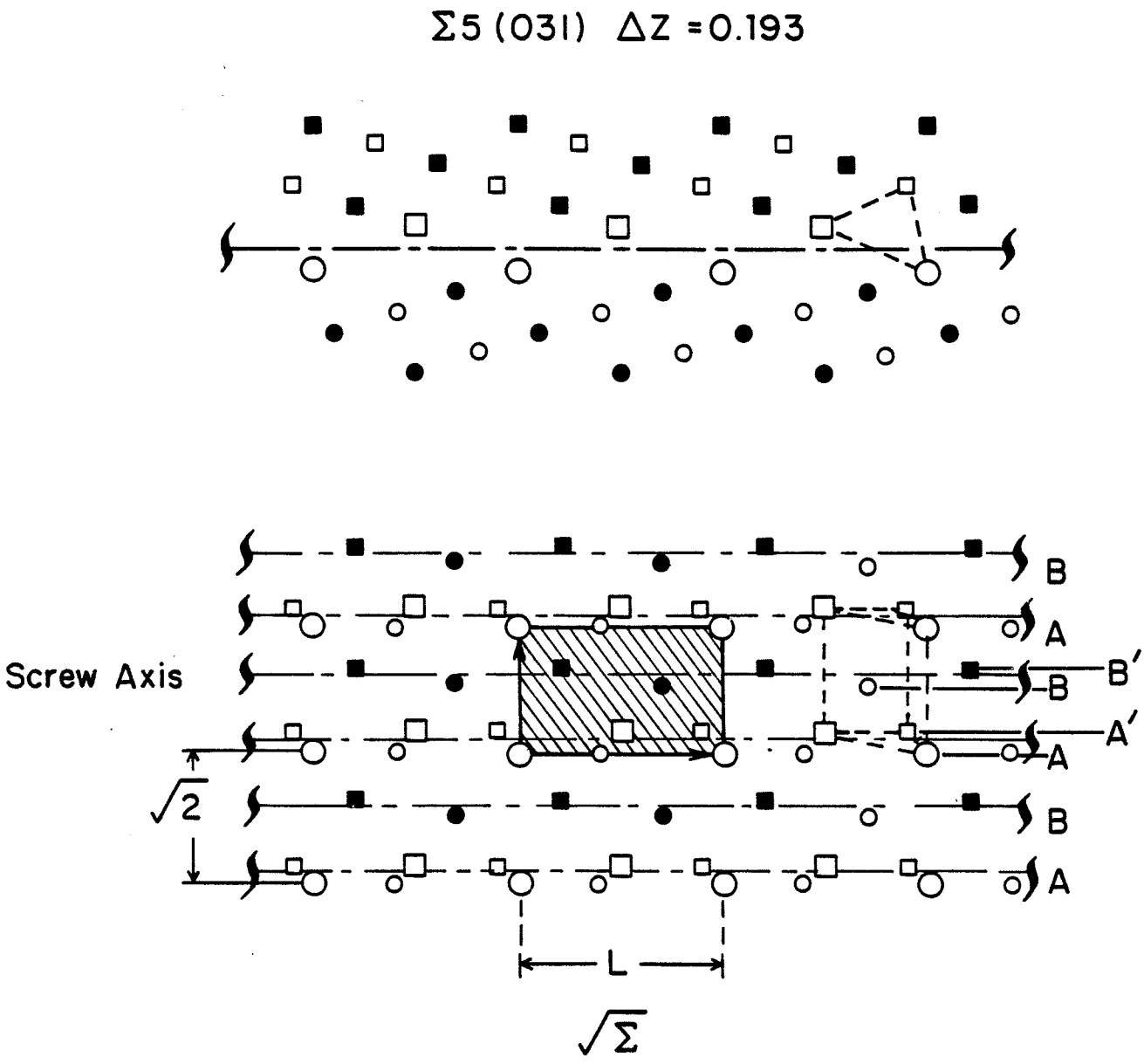


Figure 1(b) Projections of the [100] Σ5 (031) boundary structure onto a plane perpendicular to the tilt axis (top) and onto the boundary plane (bottom).

The excess volume of the boundary is then defined as:

$$V^{EX} = \frac{V^*}{A^*} = \frac{V - N\Omega}{A\Omega^{1/3}}$$

V^{EX} can be thought of as the number of atoms missing per atom in the boundary plane.

In the f.c.c. structure with spheres of unit diameter, $\Omega = 2^{-1/2}$, and $\Omega^{2/3} = 2^{-1/3}$. V^{EX} therefore represents a measurement of length, in units $\Omega^{1/3}$, which is $2^{-1/6} = 0.890899$ for our unit sphere case. If a crystal were pulled apart at a plane by $2^{-1/6}$ sphere diameters, that plane would be associated with $V^{EX} = 1.0$.

The excess volume can then be associated with the spacing between the two nearest planes parallel to the boundary in the two crystals (in the unfaceted case). The excess of that spacing over the normal spacing between such planes in each crystal (in the case of symmetric boundaries), times $2^{1/6}$, is the excess volume. It is of course possible to normalize the excess volume to other quantities, such as the sphere diameter or the unit cell edge. This is what most studies of boundary structure do when they report a translation of the crystals normal to the boundary plane.

2.4 *Determination of Interstitial and Substitutional Sites and Sizes*

Interstitial centers and sizes were determined by constructing (by numerical methods) spheres passing through all sets of four atom centers, and containing no atom center. The center of such a sphere is the center of an interstitial site, and its diameter is equal to the sum of the original sphere diameter (= 1) and the diameter of the largest sphere which would just fit into the interstitial site. The figures of Section 5 show the center locations and the diameters of the largest of these interstitials.

Substitutional sphere sites were identified and sized by a modification of this procedure: an atom was removed from the boundary, and the center and size of the largest sphere that could be re-inserted was determined as described above.

A typical boundary contains several interstitial and several substitutional sites per repeat unit. The interstitial sites shown can all be occupied at the same time without overlap between the interstitial spheres. If two overlapping sites occurred, the larger was retained and the smaller was discarded. Because of this, it is possible that a listed interstitial is in a mechanically unstable position, because the nearby stable site was eliminated by overlap of a larger site. In contrast, it is not generally possible to have all the substitutional sites occupied at the same time; putting a substitutional sphere in one site will usually exclude the possibility of putting a substitutional at a nearby site.

2.5 *Method of Identifying Boundary Structures*

The boundary structures were identified primarily by examining the topological shapes created by joining the centers of neighboring spheres between the two crystals and within each crystal. For this, the definition of neighboring spheres was extended to a spacing of $\sqrt{2}$ sphere diameters between sphere centers, and occasionally slightly beyond that. A secondary consideration was given to the number, location and nearest neighbors of the larger interstitial sites, which allows us to stretch the definition of the nearest neighbor spheres in a logical manner.

The classification of the various polyhedral structures occuring in a dense random packing of single-sized hard spheres was developed in detail by Frost [5]. It is shown there that if a nearest neighbor definition of more than $\sqrt{\frac{12}{7}} = 1.309$ sphere diameters is used, then it is possible to have the ambiguity of the same region being described by different, interpenetrating

tetrahedra. Because of the symmetry and regularity imposed by the crystals, we do not find arrangements that have interpenetrating tetrahedra near the minimum distance of $\sqrt{\frac{12}{7}}$. In the crystal, a nearest neighbor distance of $\sqrt{2}$ would cause the ambiguous definition of a regular octahedron as interpenetrating tetrahedra. For the boundary structures, however, we can use the $\sqrt{2}$ distance in those cases where it does not lead to interpenetration, and exclude it where it does. This allows us to identify structures by constructing those neighbor connections which form convenient and representative polyhedra around the interstitial sites.

For [100] and [110] tilt boundaries, the most representative polyhedron to describe the surroundings of the larger interstitial sites is usually a capped trigonal prism, aligned with the tilt axis. For a few cases, other shapes are more representative because of the number of neighbors of the interstitial sites (see Sections 4.5 - 4.7). Differentiating between different shapes can occasionally be ambiguous; since the identification is purely a matter of definition, the structure of the boundary should be considered as it stands, not as a set of idealized regular polyhedra of the same type.

3. GENERAL CONVENTIONS OF PRESENTATION

In this section we explain the various conventions we have used in the presentation of the boundaries.

3.1 *Description of Figures*

The boundaries in this catalogue are shown as projections onto a plane perpendicular to the tilt axis. The unit sphere locations are shown as different circular symbols for each different layer: open, solid, or crossed circles. Each boundary is shown twice. The left-hand figure shows the loca-

tion of the centers of the interstitial sites; the right-hand figure shows the location of the centers of the substitutional sites. The size of each site is given below the figure: "size" means the diameter of the largest hard-sphere which can be placed at the site, in units of the diameter of the spheres used to make the crystals. The site symbols are usually, but not always, repeated for each recurrence of the site in the figure. The sites are often labeled A, B, C, etc., which indicates which of the various equivalent recurrences of a site has its coordinates listed in the accompanying chart. For some boundaries there are more than five distinct interstitial or substitutional sites. In this case, the smaller sites are generally not plotted in the figure, though they are listed in the chart.

Each figure is accompanied by a numbered list of sphere coordinates, and a chart giving the size, coordinates, and neighbors of each substitutional and interstitial site. The numbers of the unit sphere neighbors of a site are occasionally given with primes or double primes (e.g. 7 , 7' or 7' , 7"). These primes refer to unit spheres that are above or below the primary layers whose coordinates are listed. Neighboring 7,7' means that sphere 7 and the sphere above (or below) sphere 7 are treated as neighbors. Neighboring 7',7" means that the sphere above and the sphere below sphere 7 are treated as neighbors; this would only occur for the substitutional site in place of sphere 7. When more than four neighboring unit spheres are listed, this is because redundancy is created by the symmetry of the crystal with respect to the site. The same meaning of primed sphere numbers is used for the list of contact pairs between the two crystals, given at the top of each chart.

3.2 *Coordinates*

The z axis is the tilt axis, which is perpendicular to the plane of the figure. The x axis is the [110] direction in crystal number one, the lower crystal. Atom number 1 is almost always at coordinates 0,0,0. For

the majority of boundaries the open circles in the lower crystal are at $z = 0$. In that case, the solid circles are at $z = 0.5$ for [110] tilt boundaries and $z = \sqrt{2}/2$ for [100] tilt boundaries. In boundaries where there is a Δz displacement across the boundary, the atoms in the upper crystal (crystal 2), are shown with an additional ring. For the [111] tilt boundaries, in crystal 1, the open circle is at $z = 0$, the solid circle is at $z = \sqrt{6}/3$, and the crossed circle is at $z = 2\sqrt{6}/3$.

For the [110] and [100] boundaries with a Δz displacement between the crystals, equivalent boundaries can be constructed with a $+\Delta z$ or a $-\Delta z$ displacement. This is because the crystals have mirror symmetry about the (100) and (110) planes. The choice of $+\Delta z$ or $-\Delta z$ is arbitrary. For [111] boundaries, the sign of Δz cannot be
there is no mirror symmetry across the (111) planes. The Δz is fixed to correspond with the stacking order of the (111) planes. The sign of Δz can be inverted if the stacking order in both crystals is also inverted. We have not used a consistent stacking order for these boundaries; the B layer (solid circles) may sit in triangles of the A layer (open circles) which point either toward or away from the boundary. This means we have been arbitrary about which layer we label the A layer, that is, in which layer we set the origin.

3.3 *Angle Labels*

The angle used to describe the [100] tilt boundaries is the minimum angle between [100] directions in the two crystals, θ. (This was the convention used by Smith, Pond and Vitek [6].) The minimum angle between [110] directions is $90° - \theta$. The misorientation between the crystals can be described by either angle of rotation. A common convention ("misorientation convention") is to use whichever angle of rotation is smallest. This would result in the same angle being used to describe both of the two symmetric tilt boundaries for a given Σ. We decided not to use the misorientation convention in order to avoid confusion in boundary identification.

For [110] tilt boundaries we have also used the angle between [100] directions. The angle between [110] directions is in this case 180° - θ.

For [111] tilt boundaries we have used for θ the minimum angle describing the rotation between the two crystals. The rotation between the crystals could also be described by 120° - θ and 120° + θ. For the set of boundaries with mirror symmetry across the boundary plane (before translation), θ is the angle between symmetric (112) directions, one in each crystal. For the other set of boundaries in which a stacking inversion is imposed on the mirror symmetry, θ is the angle between symmetric (110) directions.

For all boundaries the labeling angle is shown opening to the left of the figure.

In certain boundaries the structures (e.g. trigonal prisms) appear to be upside down from similar structures in boundaries with neighboring angles. This occurs because it is possible, given the symmetric orientation of the crystals, to have two different relative translations of the crystals that have equivalent structure but have the roles of crystal 1 and crystal 2 reversed. If one of these is chosen rather than the other, the local structures will appear as though reflected through the boundary plane (i.e. "upside down"). We have generally used relative translations which leave similar structures in boundaries of neighboring angle in the same orientation. Exceptions to this, which therefore appear to have upside down structures, are: [100] Σ37 (061), [110] Σ27 ($1\bar{1}5$), [110] Σ11 ($1\bar{1}3$), and [111] Σ7 ($2\bar{3}1$).

3.4 *Accuracy*

The interstitial and substitutional sites are listed to five decimal places of accuracy. This is justified for some of the boundaries, but it is not for certain boundaries for which the atom coordinates were only calculated to four decimal places. In addition, the program to calculate interstitial sites occasionally produced errors in the fifth, or even the fourth, decimal place. All coordinates, lengths and volumes are accurate to better than one part in a thousand.

It is entirely possible that the authors have overlooked some arrangement for some boundary that is denser than the one presented here. This is particularly true if we consider faceting. We would be grateful for any such correction, and will keep available an up-dated errata sheet.

3.5 *Order of Presentation*

The boundaries for each tilt axis are shown in order of increasing angle, not in order of increasing Σ. This allows a direct inspection of the progression of structural units that provides the progression in angle. For each tilt axis we provide a figure showing the different angles that the various boundaries make with respect to their crystals. This plot provides an index to the order of presentation of the various sigma boundaries.

Only one arrangement (the densest) for each orientation is shown in the main series that progresses in angle. For several boundaries, we included alternative, less dense, arrangements in a section at the end. The progression of structural units in the main series is occasionally interrupted by faceted boundaries which may show rather different figures than the boundaries at neighboring angles. In this case, a boundary configuration that contains figures in the series may be included in the section at the end. These additional boundaries are arranged according to increasing Σ for each tilt axis.

4. RESULTS AND CORRELATIONS

Section 5 contains the figures showing the boundaries and the interstitial substitutional sites they contain, as described in Section 3. The Table of Section 5.5 presents a summary of the information, listing the excess volume, the shortest repeat distance in the plane perpendicular to the tilt axis (L), the Δz displacement between the crystals, the diameters of the three largest interstitia and substitutionals, the internal symmetry (as described in Section 4.1), and the

of the repeat unit in the boundary plane (A). In this section we discuss the general features of those results, together with some correlations between different features.

4.1 *Symmetry*

Because all the boundaries considered here are symmetrical tilt boundaries at coincidence orientations, their structure contains the symmetry of repeated identical units. The length of repeat distance in the direction of the tilt axis is determined by the distance between equivalent planes perpendicular to the tilt axis. For [110] axis it is 1.0 sphere diameters; for [100] it is $\sqrt{2}$; and for [111] it is $\sqrt{6}$. In the direction *perpendicular* to the tilt axis, the repeat distance, L, depends on the orientation or Σ value. For [100] boundaries, which have planes (0kℓ) parallel to the boundary plane, the length is $\sqrt{\Sigma}$ when k and ℓ are both odd, and $\sqrt{2\Sigma}$ when either k or ℓ is even. (Both k and ℓ cannot be even because we could then re-express the boundary plane by dividing the indices both by 2.) For [110] boundaries, which have (hh$\bar{\ell}$) planes, the length is $\sqrt{\Sigma}$ when ℓ is odd and $\sqrt{2\Sigma}$ when ℓ is even. For [111] boundaries, the length is $\sqrt{3\Sigma}$ for those boundaries without a stacking inversion, and $\sqrt{\Sigma}$ for those boundaries with a stacking inversion.

For half the [100] boundaries and several of the [110] boundaries, each plane parallel to the boundary contains atoms on both the A and B layers. In this case, any arrangement will repeat alternatively along the boundary based first on the A layer, then on the B layer, then the A layer again, etc.. This appears as a *staggering* of boundary figures, with a reversal of A and B atoms. For [100] boundaries, (0kℓ), this occurs when k + ℓ is odd, which it is for one of each pair of boundaries for each Σ value. For [110] boundaries,

$(h\bar{h}\ell)$, this occurs when h and ℓ are both odd, which it is for one of the two boundaries for some Σ values.

For [111] boundaries, a similar staggering sometimes occurs among the A, B, and C layers. For the boundaries without a stacking inversion it occurs when Σ is not a multiple of 3 (i.e. 7,13,19,31, and 37). For those boundaries with a stacking inversion, there is no staggering of identical arrangements, even though those boundaries with Σ a multiple of 3 (i.e. 3,21, and 39) do have an atom for each layer in each plane parallel to the boundary. Because of the stacking inversion, the A, B, and C atoms do not occur along the boundary in the same order.

When this staggering is present, the smallest unit of repeating structure is not actually described (in projection onto the boundary plane) by the rectangle of the vector between equivalent atoms along the tilt axis and the vector between equivalent atoms *perpendicular* to the tilt axis. It is described by the parallelogram of the tilt axis repeat vector and a non-perpendicular vector between equivalent atoms on different layers. The difference appears clearly in Fig. 1, where the two [100] $\Sigma 5$ boundaries, (021) and (031), are shown in two projections: along the tilt axis (the usual), and perpendicular to the boundary plane. For the (021) boundary, the repeat unit is a parallelogram, in accord with its staggered arrangement.

Most of the maximum density boundaries that do not have staggering show another sort of symmetry internal to the repeat unit. The arrangement of atoms in one half of the repeat unit is repeated in the other half with a rotation of 180° about an axis lying in the boundary plane, perpendicular to the tilt axis. This rotation plus translation provides a two-fold screw axis. If there is no Δz displacement between the two crystals, the rotation symmetry may degenerate into glide-reflection symmetry with the boundary

plane as the glide plane. Examples of this, in an arrangement of maximum density, are $\Sigma 3$ $(1\bar{1}2)$, $\Sigma 17b$ $(3\bar{3}4)$, and $\Sigma 43$ $(5\bar{5}6)$. For one boundary, $\Sigma 17b$ $(2\bar{2}3)$, the glide direction is not perpendicular to the tilt axis, but has a component along the tilt axis that shifts the arrangement from the A layer to the B layer, etc..

For boundaries with internal screw axis symmetry, the axis is always in the plane of the boundary, that is, midway between the last planes present in the two crystals. There are two axes per tilt axis repeat vector. For the degenerate case without staggering, e.g. $\Sigma 3$ $(1\bar{1}2)$ the axes are in the planes of the A and B layers. For the degenerate case with staggering, e.g. $\Sigma 17b$ $(2\bar{2}3)$, they are midway betwen the A and B layers. For the non-degenerate cases, i.e. $\Delta z \neq 0$, they are either midway between the A and A' layers and midway between the B and B' layers, or midway between the A and B' layers and B and A' layers. (We are labeling as A' the layer in crystal 2 which is nearest to the A layer in crystal 1.) In the former case, a given local arrangement stays at the A - A' and A' - A level. In the latter, an arrangement appears to stagger between the A - A' level and the B' - B level.

Nine of the boundary configurations are in exact coincidence site lattice (CSL) positions, as marked in the table. This means that $\Delta z = 0$. For four boundaries, they are not the densest arrangement. When a boundary is in the exact CSL position, the two crystals are in exact mirror symmetry, except for a few atoms per repeat unit, near the boundary plane. The configuration can sometimes be made entirely symmetrical by moving those atoms into the minor plane without a change in density. An example of this are the $\Sigma 25a$ (071), and the $\Sigma 9$ $(1\bar{1}4)$ boundaries. The latter boundary can also be made into a faceted boundary with glide reflection symmetry by a different rearrangement of a small number of atoms at constant density.

TABLE 1

Faceted Boundaries

Tilt Axes	Boundary	Boundary Angle	Dense Nearly Parallel Planes*	Ideal Boundary Angle♦	V^{EX} Faceted	V^{EX} Unfaceted
[100]	Σ17a (053)	61.93°	(100) (210)	63.43°	0.40339	0.42850
	Σ29a (073)	46.40°	(110) (100)	45.00°	0.39735	0.46398
	Σ29a (052)	43.60°	(110) (100)	45.00°	0.39336	0.4422
	Σ85 (0,11,7)	64.94°	(110) (310)	63.43°	0.37085	†
[110]	Σ19a ($1\bar{1}6$)	153.47°	(100) (311)	154.76°	0.42619	0.4498‡
	Σ27a ($\bar{5}\bar{5}2$)	31.58°	(110) (111)	35.26°	0.31195	0.43619
	Σ33a ($1\bar{1}8$)	159.95°	or (211) (511) / (100) (151)	160.53° / 164.21°	0.42017	†
	Σ33c ($2\bar{2}5$)	121.01°	(100) (111)	125.26°	0.30932	0.41450‡
	Σ41c ($3\bar{3}8$)	124.12°	(100) (111)	125.26°	0.27305	0.46822‡
[111]	Σ39a (341)	32.21°	($1\bar{1}0$) ($1\bar{2}1$)	30.00°	0.45379	†
	Σ37c (10,$\bar{1}\bar{1}$,1)	50.57°	**		0.46030	†
	Σ31a (7,$\bar{1}\bar{1}$,4)	17.90°	**		0.49153	†
	Σ21a ($2\bar{3}1$)	21.79°	**		0.49375	†
	Σ13b ($5\bar{7}2$)	27.80°	($1\bar{1}0$) ($1\bar{2}1$)	30.00°	0.48069	†

* Planes parallel to the tilt axis
** None apparent
† No unfaceted configuration calculated
‡ Unfaceted configuration without symmetry
♦ Boundary angle that would have the dense planes exactly parallel

The only boundaries that do not show staggering, screw axis, or potential mirror symmetry in their densest arrangements are [111] boundaries without stacking inversion where Σ is a multiple of three: Σ39a ($5\bar{7}2$), Σ21a ($4\bar{5}1$), and Σ3 ($1\bar{2}1$). The boundary Σ3 ($1\bar{2}1$) shows no internal symmetry as a [111] boundary, but does have glide-reflection symmetry as a [110] boundary, ($1\bar{1}2$).

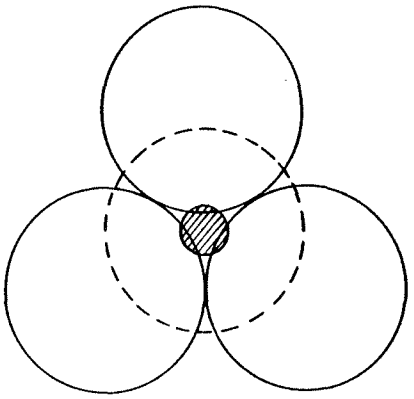
The common occurence of screw axis symmetry is a surprising result of this catalogue. Were it not for the Σ25a (071) boundary, we might conjecture that all [100] and [110] boundaries showed either staggering or screw axis symmetry in their densest arrangement.

4.2 *Faceting*

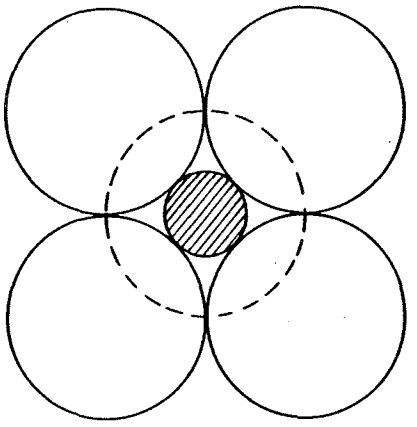
That some boundaries can be constructed more densely in a faceted configuration is a surprising result of this study. As mentioned in Section 2.2, this occurs for [100] and [110] tilt boundaries when there is a dense plane, A, in crystal one that is nearly parallel to a dense plane, B, in crystal two. Because of the symmetry, plane B of crystal one is also almost parallel to plane A of crystal two. This situation will not lead to faceting, however, if planes A and B make too great an angle with the boundary plane. Table 1 lists all the faceted configurations we have discovered, together with their dense nearly parallel planes and the excess volume of the faceted and unfaceted configurations.

4.3 *Excess Volume*

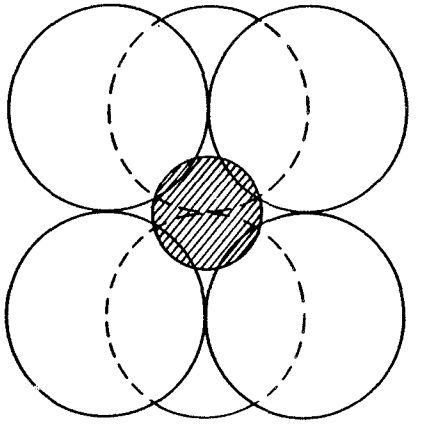
The excess volumes vary from zero (for the coherent twin) to about 0.5. In general [110] tilt boundaries are the densest, with an average excess volume, v^{EX}, of 0.309 (including the coherent twin). The [100] tilt boundaries are less dense, with an average v^{EX} of 0.422 (including Σ85b $(0,\bar{1}\bar{1},7)$). The [111] tilt boundaries are less dense still; those without a stacking inversion have v^{EX} averaging 0.419 if the Σ3 ($1\bar{2}1$) boundary is included, which is also a [110] boundary. Without the Σ3, they have an average of 0.449. The [111] boundaries with a stacking inversion have an average v^{EX} of 0.463.



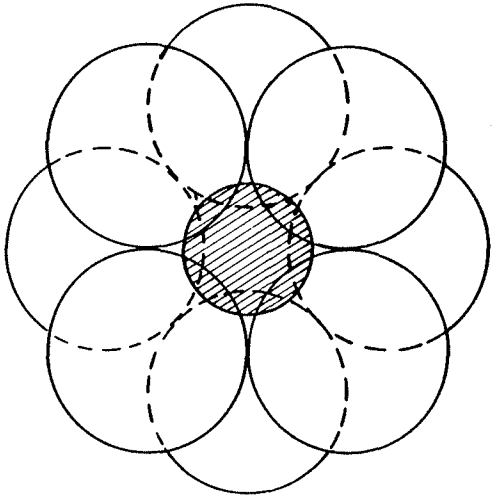
TETRAHEDRON
0.2248



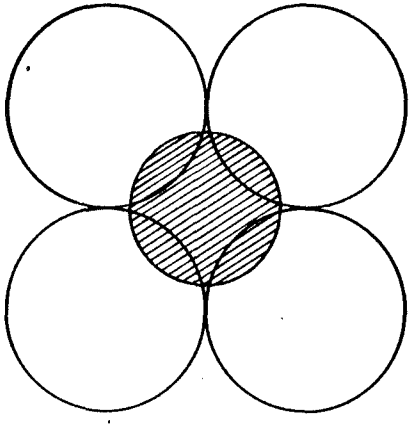
OCTAHEDRON
0.4142



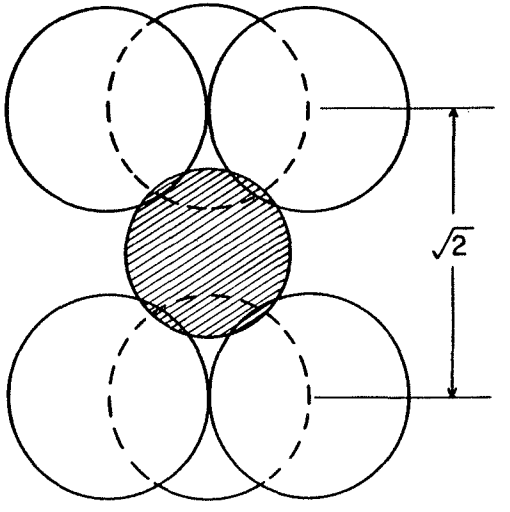
TRIGONAL PRIM
0.5276



SQUARE ANTIPRISM
0.6454



CUBE
0.7321



STRETCHED TRIGONAL PRISM
0.8257

Figure 2 Interstitial sites in various regular polyhedra.

TABLE 2

Interstitials in Undistorted Polyhedra

Polyhedron	Diameter of largest interstitial sphere
Tetrahedron	0.2247
Octahedron	0.4142
Regular Trigonal Prism (with or without capping spheres)	0.5275
Square Antiprism	0.6454
Cube	0.7320
Stretched Trigonal Prism (height = $\sqrt{2}$, without capping spheres.)	0.8257

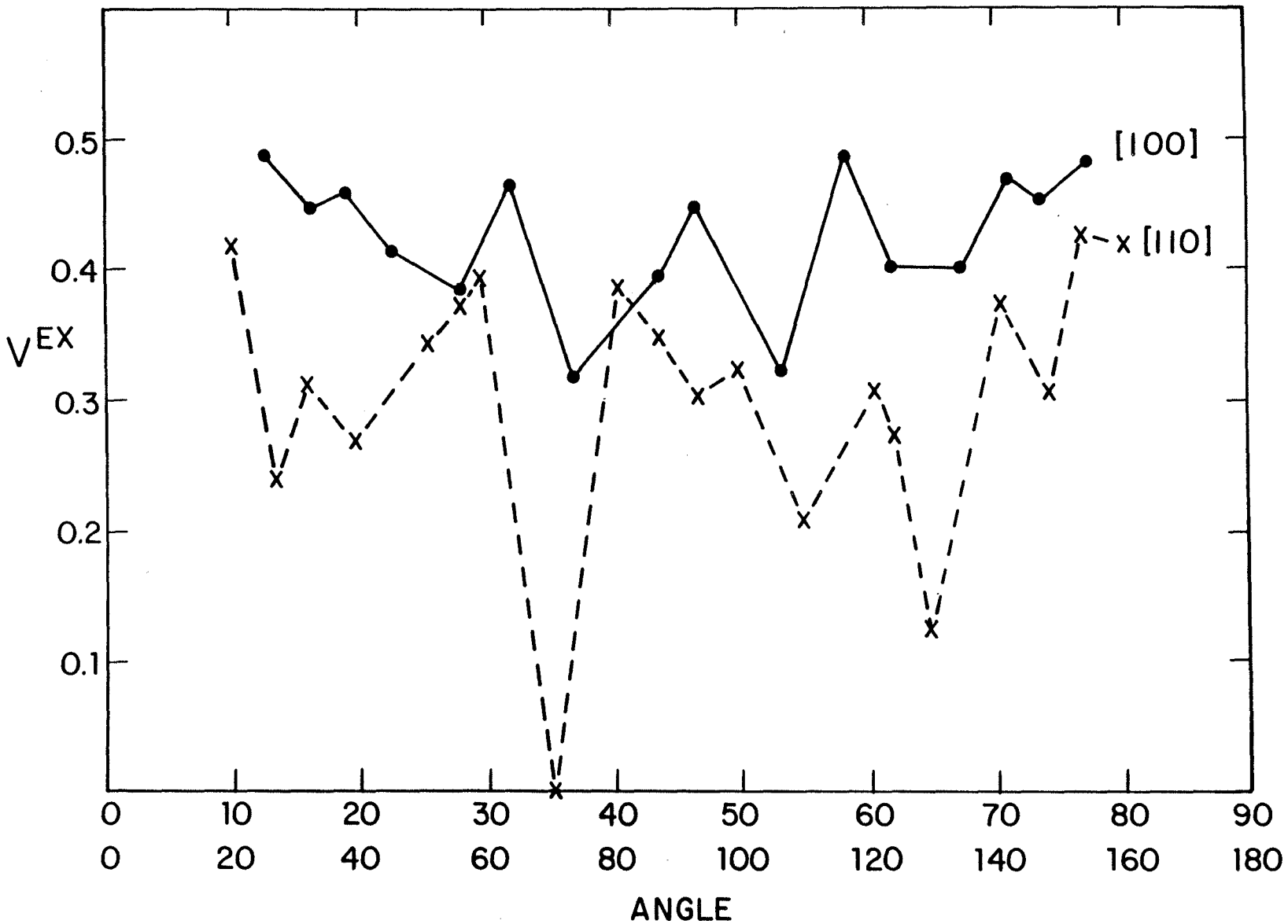


Figure 3 Excess volume versus angle for [100] and [110] boundaries.

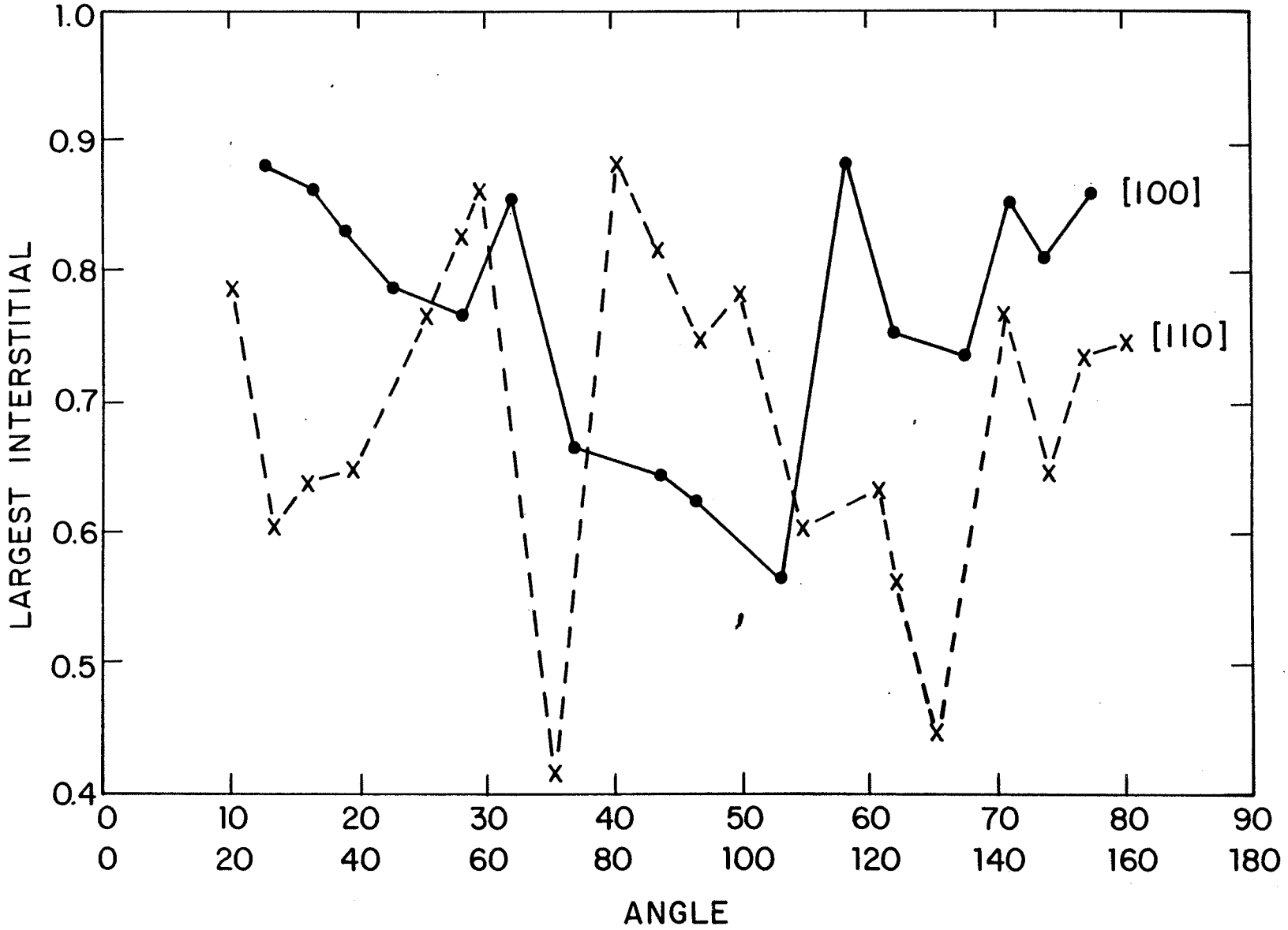


Figure 4 Largest interstitial versus angle for [100] and [110] boundaries.

In general the boundaries with higher Σ have greater excess volume, for all tilt axes. The correlation is only rough, and is not plotted. The best correlation we have found for all the boundaries together is with the area of the repeat unit. This is shown in Fig. 5, and replaces the correlation with repeat distance published previously [4]. (In that reference the repeat distance used for boundaries showing staggering internal symmetry was the projection of the repeat unit vector onto the plane perpendicular to the tilt axes, which is 1/2 L.)

To demonstrate the general validity of the correlation between excess volume and tilt axis, Fig. 3 plots the excess volume versus angle for [100] and [110] boundaries. With a similar number of boundaries for each axis, the [110] boundaries are definitely denser on average.

4.4 *Interstitial and Substitutional Sites*

Almost all boundaries contain interstitials of diameter 0.6 or larger; many contain interstitials greater than 0.8 in diameter. Interstitials larger than0.90 are not found in boundaries arranged in their densest configurations. These interstitials are much larger than those found either in the perfect crystal (maximum 0.414) or in the dense random packing of hard spheres (maximum 0.7; see Frost [5]). For comparative purposes, Table 2 lists the interstitial sizes in several undistorted polyhedra. Figure 2 shows these polyhedra with unit spheres and shaded interstitials.

The size of the largest interstitial correlates roughly with the Σ value of the boundary. A better correlation is obtained between the largest interstitial and the area of the boundary repeat unit, shown in Fig. 5. For a given repeat unit area, in the densest configuration, there is a maximum interstitial size possible. If the site were too large, then the boundary

could be densified by pulling the crystals apart until the site reached 1.0, and inserting another unit sphere. We have not developed a general method for calculating this maximum.

When all the boundaries are considered, there does not appear to be any consistent variation in largest interstitial size with tilt axis. This is shown in Fig. 4 which plots the largest interstitial size against angle for [100] and [110] boundaries.

Certain boundaries which are particularly dense contain no special substitutional sites, that is, no sites larger than 1.0. All unit spheres are constrained in all directions by contacts with other spheres.

Other boundaries with larger excess volume contain large substitutional sites of size up to 1.23. The correlation between excess volume and largest substitutional is very rough. The correlation between repeat unit area and largest substitutional size (shown in Fig. 5) is also rough.

4.5 *[100] Tilt Boundary Structures*

All the [100] tilt boundaries contain trigonal prisms, which, because they must conform to the spacing of (100) planes, are extended to a height (normal to the figure) of $\sqrt{2}$ instead of 1. (See the stretched trigonal prism in Fig. 2.) When there is a Δz displacement between the crystals, the trigonal prisms are distorted by a shear in the plane of the boundary. The prisms are usually distorted by stretching one or two of the horizontal edges between the two crystals. The only exceptions to this are $\Sigma 5$ (021), $\Sigma 13$ (023), and the third densest configuration of $\Sigma 29$ (073).

Because the trigonal prism are stretched to $\sqrt{2}$ height, the spheres on the alternate plane which form the caps to the rectangular faces are much closer to the center than for a regular capped trigonal prism. Two

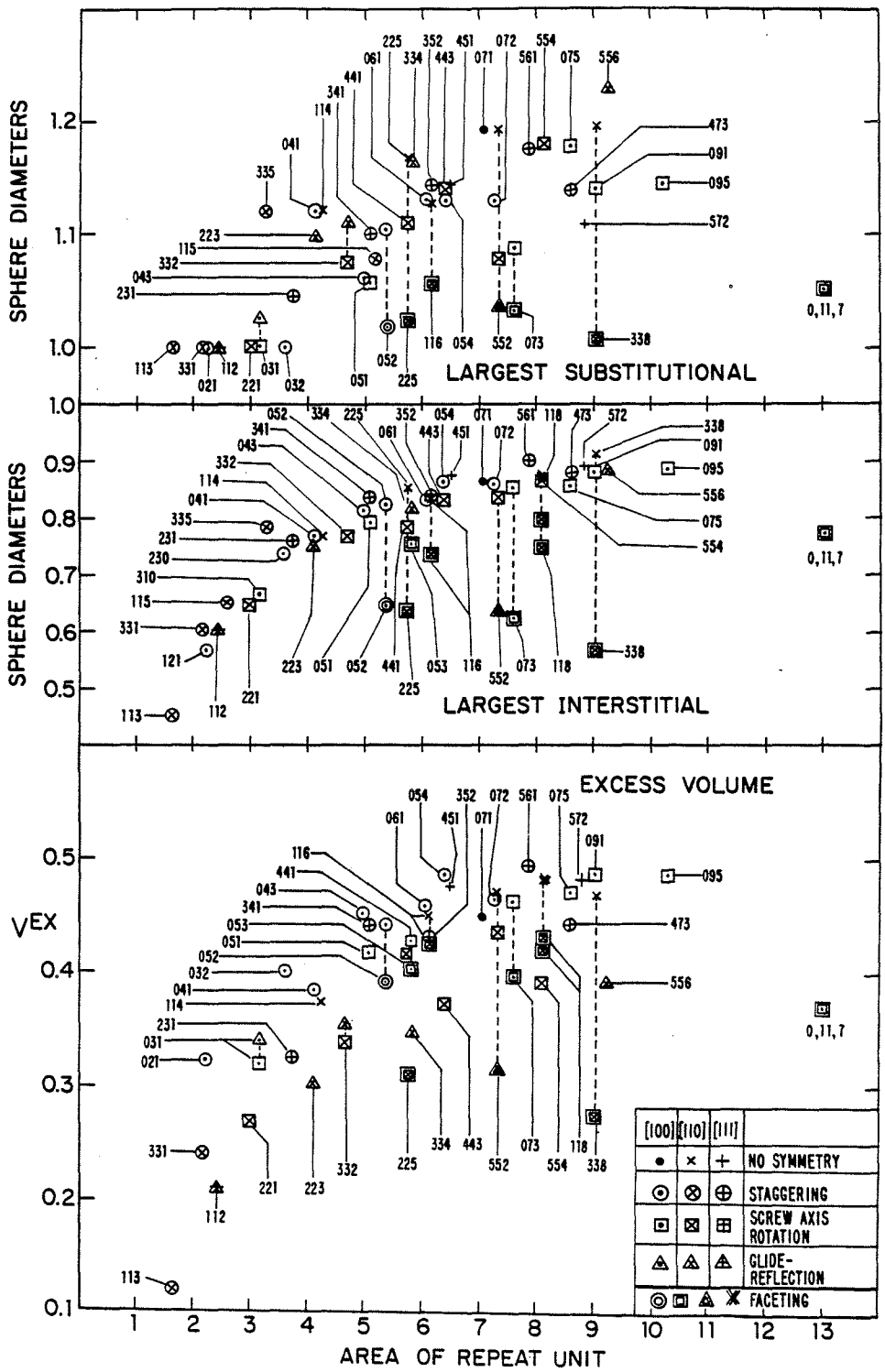


Figure 5(a) Excess volume, largest interstitial and largest substitutional versus area of boundary repeat unit.

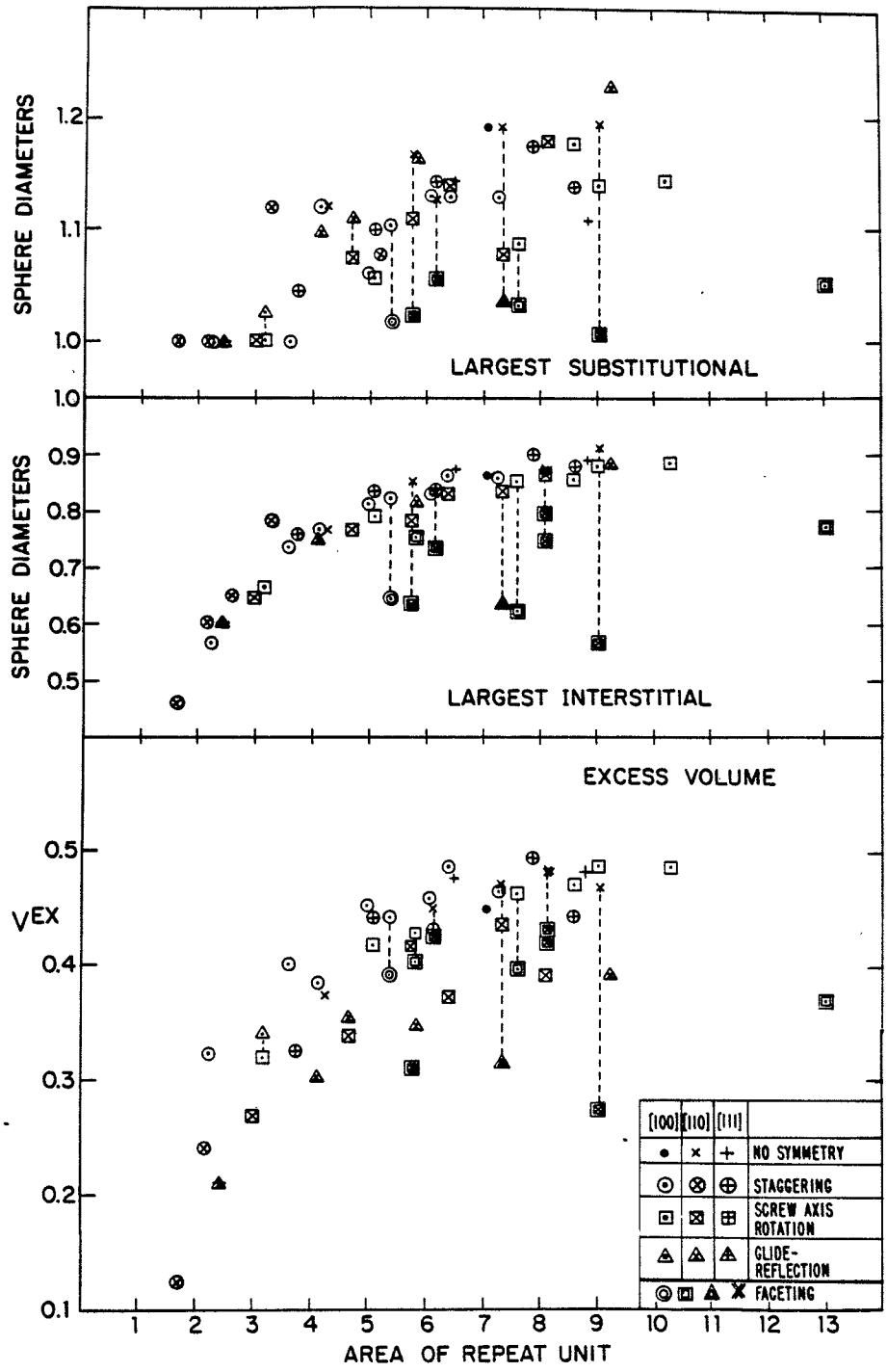


Figure 5(b) Same as Figure 5(a) with the labels removed for clarity.

caps may be as close to each other as 1.366, which is less than the prism height. (All three caps cannot mutually be as close as this, because the crystal symmetry does not allow it.) The interstitial site in the middle of a prism is always limited in size by one or more of the capping spheres. The interstitial never touches all six corners of the prism. If the prism is sheared by a Δz displacement, the interstitial could touch at most five prism corners, but never does so because it is limited by a capping sphere. Often the interstitial does not lie in the midplane of the prism (the plane of the caps), but closer to one end or the other. (With a Δz displacement where not all the capping atoms are in the same (100) plane, the interstitial often does not lie in the plane of the caps in either crystal.)

The prisms are linked by other figures. In some boundaries, the only other figures are octahedra and tetrahedra, more or less distorted (they are not outlined on the figures). But in some boundaries other figures appear. In various configurations of boundaries with angles greater than 61° there appears a shape which we may call the five-sided channel of type A. (It is not marked in Σ13 (032) and Σ85 (0,11,7), and appears only in the less dense configurations of Σ37a (075) and Σ17a (053).) It is an almost cylindrical channel ringed by five atoms with the stacking sequence A-A-A-B-B. A clear example appears in Σ25 (043). Another such five-sided channel is possible (type B) with the stacking sequence A-B-A-B-A; it is a distortion of a trigonal prism which appears in some [110] boundaries, but not in any of the [100] boundaries.

4.6 *[110] Tilt Boundary Structures*

The $\Sigma 3$ $(1\bar{1}1)$ boundary is the coherent twin, containing only undistorted octahedra and tetrahedra. Most of the others contain trigonal prisms (some of which are capped with half-octahedra). The spacing of the [110] planes is 1.0, so the figures are not stretched normal to the plane of the figure. In those boundaries with a Δz displacement, the trigonal prisms are distorted by a shear in the plane of the boundary. In general, the prisms are distorted by a stretching in the plane of the figure. Those seven boundaries with angles less than 59°, $(4\bar{4}1)$ to $(5\bar{5}4)$, have one of the horizontal edges stretched to $\sqrt{2}$ between two spheres in the same crystal. For some of these, another edge (between the two crystals) is stretched beyond $\sqrt{2}$.

The five boundaries between 80° and 110°, $(5\bar{5}6)$ to $(1\bar{1}2)$, have a horizontal edge between the crystals stretched to $\sqrt{2}$. These boundaries make contact between the two crystals in a similar arrangement, which also produces $\Delta z = 0$.

The five boundaries with angles between 121° and 149°, $(2\bar{2}5)$ to $(1\bar{1}5)$ show more nearly regular trigonal prisms. The boundary with the greatest angle, 159.95°, $\Sigma 33a$ $(1\bar{1}8)$, shows no trigonal prism at all in its densest, faceted, arrangement.

Because the trigonal prisms are of height 1.0, the capping spheres can be far enough from the center to allow the interstitial site to touch all six ($\Delta z = 0$) or five of the six ($\Delta z \neq 0$) prism corners. This is the case for boundaries of angle greater than 121° which show nearly regular prisms. In other boundaries, however, the horizontal stretching of prism edges to $\sqrt{2}$ brings the capping spheres closer to the center and they begin to limit the interstitial size. For boundaries with prisms stretched $\sqrt{2}$ across the boundary (80° to 110°), the interstitial touches two pairs of prism corners

and one cap (except for $\Sigma 43$ $(3\bar{3}5)$ where it touches all six corners). For boundaries with prisms stretched $\sqrt{2}$ within one crystal (less than 59°), the interstitial touches either three different corners and one cap, or two corners and two caps.

In addition to trigonal prisms, five-sided channels appear in several [110] boundaries. The four boundaries with angles greater than 141° all have an example of a five-sided channel of type A. Although some of the regions drawn as channels in these boundaries might also be considered widely stretched trigonal prisms, each boundary shows at least one channel that cannot be well described as a prism.

Five-sided channels of type B are found in two of the [110] boundaries: $\Sigma 19$ $(3\bar{3}1)$ 26.53°, and the less dense configuration of $\Sigma 9$ $(2\bar{2}1)$ 38.94°. The channel description is more appropriate than the prism description because the channels contain two different interstitial sites.

4.7 *[111] Tilt Boundary Structures*

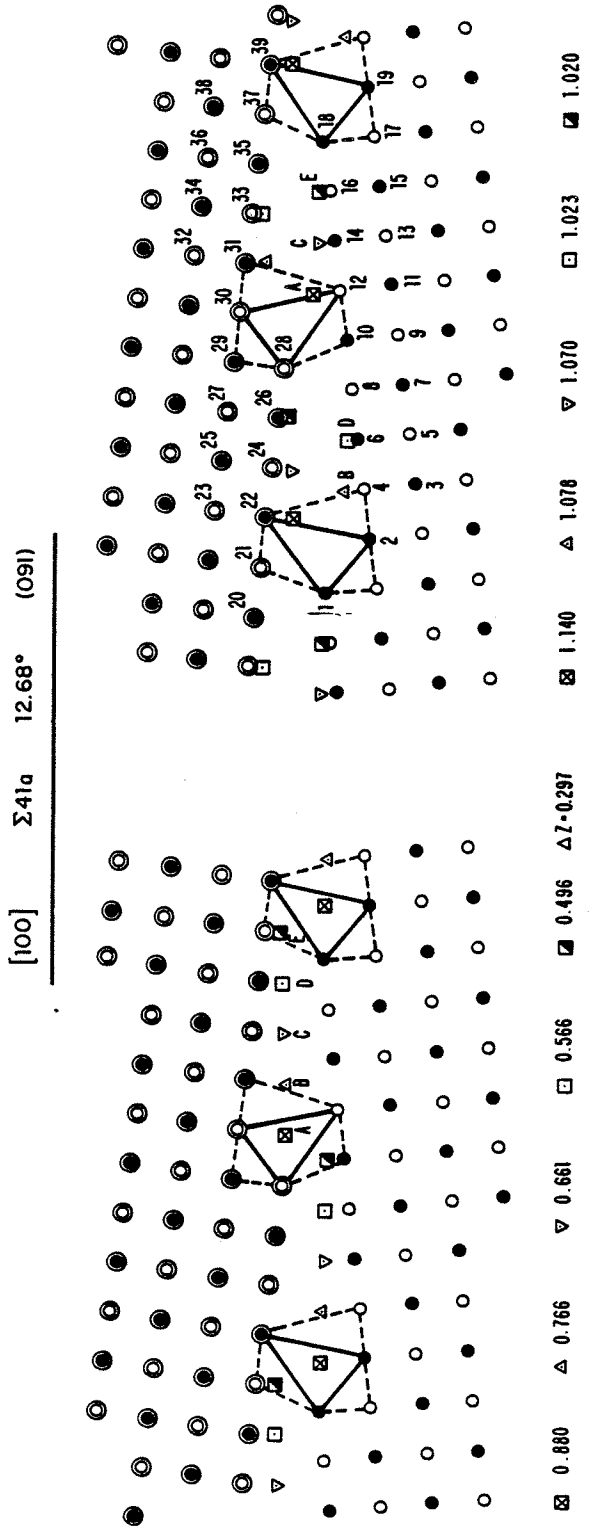
Because the spacing between identical layers of the (111) planes is $\sqrt{6}$, there appear no trigonal prisms that have the tilt axis as their vertical direction. The triangles drawn between the crystals show contacts or near contacts between the crystals within one layer (offset by Δz). For all the [111] boundaries without a stacking inversion, and some with a stacking inversion, the triangles delineate tetrahedra. Neighboring the delineated tetrahedra, there are other tetrahedra which are more distorted. The number of these additional tetrahedra depends on the distortion allowed in the definition of a tetrahedron (or the nearest neighbor distance).

The spaces between the tetrahedra cannot be conveniently classified as simple shapes. They form multi-faceted channels running in the direction of the tilt axis, zig-zagging back and forth between the different (111) planes.

5. CATALOGUE OF BOUNDARY STRUCTURES

5.1 DENSEST [100] BOUNDARIES

Listed in order of increasing angle



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	2.00000	0.00000	0.00000
4	1.50000	0.50000	0.70711
5	2.50000	0.50000	0.70711
6	2.00000	1.00000	0.00000
7	3.00000	1.00000	0.00000
8	2.50000	1.50000	0.70711
9	3.50000	1.50000	0.70711
10	3.00000	2.00000	0.00000
11	4.00000	2.00000	0.00000
12	3.50000	2.50000	0.70711
13	4.50000	2.50000	0.70711
14	4.00000	3.00000	0.00000
15	5.00000	3.00000	0.00000
16	4.50000	3.50000	0.70711
17	5.50000	3.50000	0.70711
18	5.00000	4.00000	0.00000
19	6.00000	4.00000	0.00000
20	-0.80759	0.50949	-0.29703
21	-0.21003	0.88754	0.41008
22	0.38753	1.26558	-0.29703
23	0.00948	1.86315	0.41008
24	0.98509	1.64363	0.41008
25	0.60704	2.24119	-0.29703
26	1.58265	2.02168	-0.29703
27	1.20460	2.61924	0.41008
28	2.18021	2.39973	0.41008
29	1.80216	2.99729	-0.29703
30	2.39972	3.37534	0.41008
31	2.99728	3.75339	-0.29703
32	2.61924	4.35095	0.41008
33	3.59485	4.13144	0.41008
34	3.21680	4.72900	-0.29703
35	4.19241	4.50949	-0.29703
36	3.81436	5.10705	0.41008
37	4.78997	4.88754	0.41008
38	4.41192	5.48510	-0.29703
39	5.38753	5.26559	-0.29703

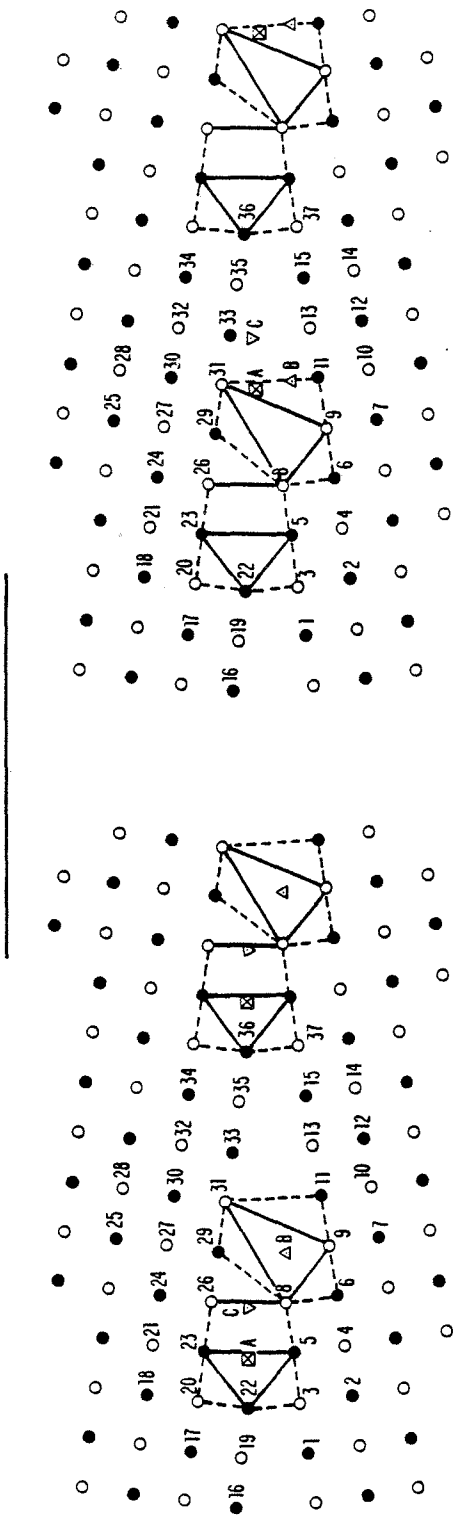
[100] Σ41a 12.68° (091) Δz = -0.29703

V^{EX} = 0.48695

Contacts: 1-20, 1-21, 8-28, 10-28

Interstitials	x	y	z	d	Touching
A	2.73067	2.85055	-0.29612	0.88006	10,12,29,30,(30',31)
B	3.27993	3.30285	0.41209	0.76639	12,14,30,31
C	3.82765	3.76344	-0.29703	0.66086	16,31,33,33',35
D	4.37219	4.22532	0.41008	0.56598	18,33,35,35',37
E	4.92019	4.68171	-0.29703	0.49576	18,35,37,37',39

Substitutionals		x	y	z	d	Touching
A	12	3.23045	2.76955	0.70711	1.14039	10,10',14,14',30
B	4	1.30065	0.69935	0.70710	1.07796	2,2',6,6',24
C	14	3.81172	3.18828	0.0	1.06968	12,12',16,16',31
D	6	1.89359	1.10641	0.0	1.02252	4,4',8,8',26
E	16	4.40035	3.59965	0.70711	1.01976	14,14',18,18',33



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.0	0.	0.0
3	0.5	0.5	0.70711
4	1.5	0.5	0.70711
5	1.0	1.0	0.0
6	2.0	1.0	0.0
7	3.0	1.0	0.0
8	1.5	1.5	0.70711
9	2.5	1.5	0.70711
10	3.5	1.5	0.70711
11	3.0	2.0	0.0
12	4.0	2.0	0.0
13	3.5	2.5	0.70711
14	4.5	2.5	0.70711
15	4.0	3.0	0.0
16	-1.24	0.32	0.0
17	-0.96	1.28	0.0
18	-0.68	2.24	0.0
19	-0.62	0.66	0.70711
20	-0.34	1.62	0.70711
21	-0.06	2.58	0.70711
22	0.0	1.0	0.0
23	0.28	1.96	0.0
24	0.56	2.92	0.0
25	0.84	3.88	0.0
26	0.90	2.30	0.70711
27	1.18	3.26	0.70711
28	1.46	4.22	0.70711
29	1.52	2.64	0.0
30	1.80	3.60	0.0
31	2.14	2.98	0.70711
32	2.42	3.94	0.70711
33	2.76	3.32	0.0
34	3.04	4.28	0.0
35	3.38	3.66	0.70711
36	4.00	4.00	0.0
37	4.5	3.5	0.70711

[100] $\Sigma 25a$ 16.26° (071) $\Delta z = 0.0$

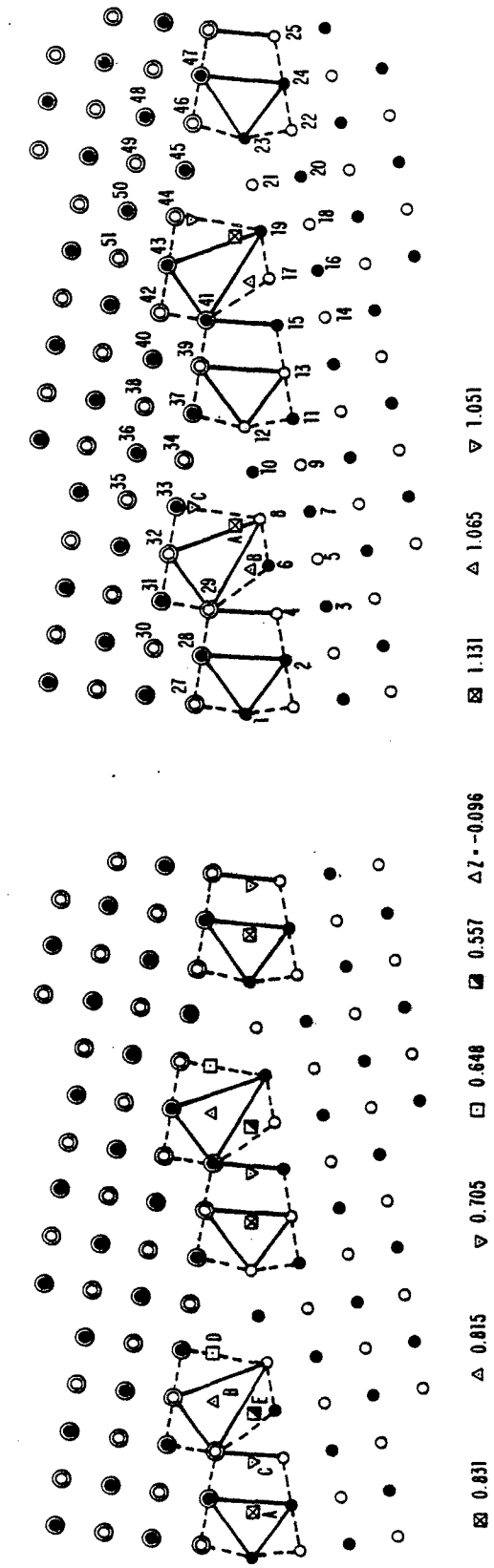
$v^{EX} = 0.4490$

Contacts: 1-22, 3-22, 5-22, 8-26

Interstitials		x	y	z	d	Touching
	A	0.57143	1.42857	0.70711	0.86263	3,5,5',8,20,23,23',26
	B	2.08490	1.91509	0.0	0.83805	6,9,9',11,29
	C	1.14286	1.85714	0.0	0.73793	5,8,8',23,26,26',29
	(D)	2.78571	2.64286	0.40406	0.57791	11,13,31,33
	(E)	3.26923	2.73077	0.0	0.55757	11,13,13',15,33
	(F)	3.46774	3.5	0.0	0.46054	33,35,35',36,15
	(G)	3.87500	3.12500	0.70711	0.45774	13,15,15',37,35

Substitutionals		x	y	z	d	Touching
A	31	2.35577	2.58654	0.70711	1.19214	9,29,29',33,33'
B	11	2.74359	2.25641	0.0	1.12743	9,9',13,13',33
C	33	2.91111	3.04444	0.0	1.09644	11,31,31',35,35'
(D)	13	3.35937	2.64063	0.70711	1.03917	11,11',15,15',35
(E)	29	2.0	2.16216	0.11467	1.03906	8,9,11,31
(F)	35	3.46053	3.51316	0.70711	1.02785	13,33,33',36,36'

Lattices exactly on the coincidence lattice; CSL sites: 22,36



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	2.00000	0.00000	0.00000
4	1.50000	0.50000	0.70711
5	2.50000	0.50000	0.70711
6	2.00000	1.00000	0.00000
7	3.00000	1.00000	0.00000
8	2.50000	1.50000	0.70711
9	3.50000	1.50000	0.70711
10	3.00000	2.00000	0.00000
11	4.00000	2.00000	0.00000
12	3.50000	2.50000	0.70711
13	4.50000	2.50000	0.70711
14	5.50000	2.50000	0.70711
15	5.00000	3.00000	0.00000
16	6.00000	3.00000	0.00000
17	5.50000	3.50000	0.70711
18	6.50000	3.50000	0.70711
19	6.00000	4.00000	0.00000
20	7.00000	4.00000	0.00000
21	6.50000	4.50000	0.70711
22	7.50000	4.50000	0.70711
23	7.00000	5.00000	0.00000
24	8.00000	5.00000	0.00000
25	8.50000	5.50000	0.70711
26	-0.89616	0.43390	-0.09288
27	-0.26102	0.74471	0.61422
28	0.37411	1.05552	-0.09288
29	1.00925	1.36633	0.61422
30	0.06330	1.69066	0.61422
31	0.69843	2.00147	-0.09288
32	1.33357	2.31228	0.61422
33	1.96870	2.62309	-0.09288
34	2.60384	2.93390	0.61422
35	1.65789	3.25823	0.61422
36	2.29303	3.56904	-0.09288
37	3.23897	3.24471	-0.09288
38	2.92816	3.87985	0.61422
39	3.87411	3.55552	0.61422
40	3.56330	4.19066	-0.09288
41	4.50924	3.86634	-0.09288
42	4.19843	4.50147	0.61422
43	4.83357	4.81228	-0.09288
44	5.46870	5.12309	0.61422
45	6.10384	5.43390	-0.09288
46	6.73897	5.74471	0.61422
47	7.37411	6.05553	-0.09288
48	6.42816	6.37985	-0.09288
49	5.79303	6.06904	0.61422
50	5.15789	5.75823	-0.09288
51	4.52276	5.44742	0.61422

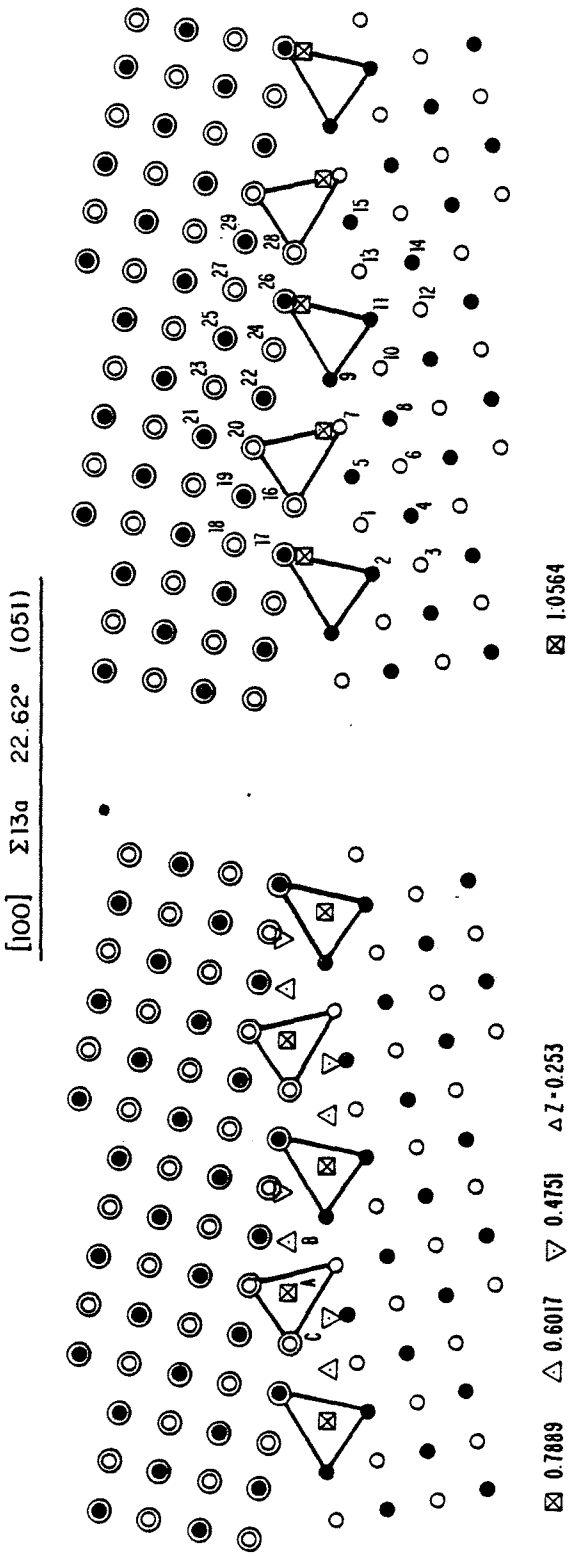
[100] Σ37a 18.92° (061) $\Delta Z = -0.09288$

$$V^{EX} = 0.45906$$

Contacts: 1-26, 1-27, 4-29

Interstitials	x	y	z	d	Touching
A	0.58697	0.41157	0.70608	0.83141	2,28,27,unnumbered 11,13,37,39
B	1.58369	1.80116	-0.09289	0.81527	6,31,32,32',34
C	1.17535	0.82118	-0.00246	0.67939	2,4,28,29
D	2.15486	2.24270	0.61421	0.64845	8,32,33,33',34
E	1.76994	1.23006	0.70711	0.55673	4,6,6',8,29
(F)	2.79785	2.20215	0.70711	0.52542	8,10,10',12,34
(G)	2.72051	2.69549	-0.09289	0.51056	10,33,34,34',37
(H)	3.43469	2.56530	0.0	0.42622	10,12,12',37
(I)	3.27582	3.16943	0.61423	0.42411	12,34,37,37',39

Substitutionals		x	y	z	d	Touching
A	8	2.23999	1.76002	0.70711	1.13093	6,6',10,10',32
B	6	1.81834	1.18166	0.0	1.06494	4,4',8,8',29
C	33	2.06860	2.41895	0.09289	1.05100	10,32,32',34,34'
(D)	10	2.86084	2.13916	0.0	1.03836	8,8',12,12',33
(E)	28	0.44780	0.90496	-0.09289	1.02790	1,27,27',29,29'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.50000	0.70711
3	0.00000	-1.00000	0.00000
4	0.50000	-0.50000	0.70711
5	0.50000	0.50000	0.70711
6	1.00000	0.00000	0.00000
7	1.00000	1.00000	0.00000
8	1.50000	0.50000	0.70711
9	1.50000	1.50000	0.70711
10	2.00000	1.00000	0.00000
11	2.50000	1.50000	0.70711
12	3.00000	1.00000	0.00000
13	3.00000	2.00000	0.00000
14	3.50000	1.50000	0.70711
15	3.50000	2.50000	0.70711
16	-0.28330	0.92495	0.25339
17	-0.93715	0.65572	-0.45372
18	-1.20638	1.30957	0.25339
19	-0.55253	1.57880	-0.45372
20	0.10132	1.84803	0.25339
21	-0.16791	2.50187	-0.45372
22	0.75516	2.11726	-0.45372
23	0.48593	2.77111	0.25339
24	1.40901	2.38649	0.25339
25	1.13978	3.04034	-0.45372
26	2.06286	2.65572	-0.45372
27	1.79362	3.30957	0.25339
28	2.71670	2.92495	0.25339
29	2.44747	3.57880	-0.45372

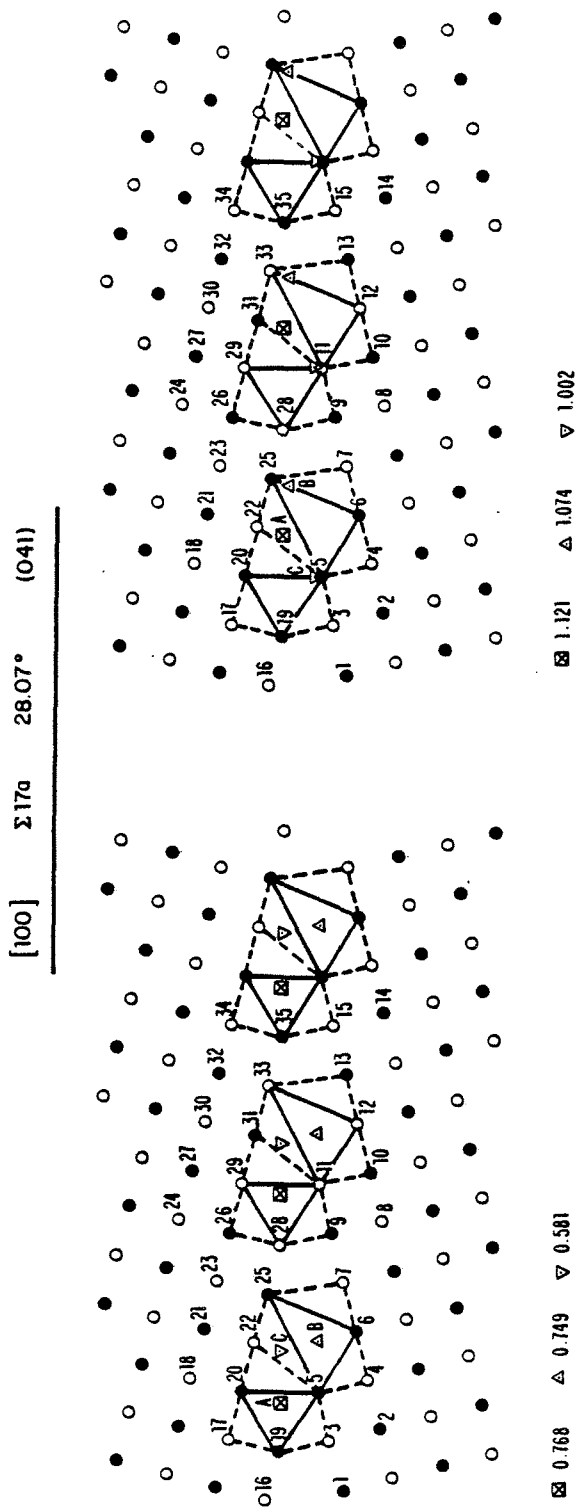
[100] $\Sigma 13\,a$ 22.62° (051) $\Delta Z = 0.25339$

$V^{EX} = 0.41761$

Contacts: 1-16, 5-16, 9-22, 9-24

Interstitials	x	y	z	d	Touching
A	0.30863	1.33705	0.95764	0.78891	5,7,19,20
B	0.89669	1.75497	0.24631	0.60166	7,9,20,22
C	0.35171	0.64829	0.0	0.47510	1,5,5',7,16

Substitutionals		x	y	z	d	Touching
A	7	1.16917	0.0	1.02822	1.05644	5,5',9,9',20



	X	Y	Z
1	0.0	0.0	0.0
2	1.0	0.0	0.0
3	0.5	0.5	0.70711
4	1.5	0.5	0.70711
5	1.0	1.0	0.0
6	2.0	1.0	0.0
7	2.5	1.5	0.70711
8	3.5	1.5	0.70711
9	3.0	2.0	0.0
10	4.0	2.0	0.0
11	3.5	2.5	0.70711
12	4.5	2.5	0.70711
13	5.0	3.0	0.0
14	6.0	3.0	0.0
15	5.5	3.5	0.70711
16	-0.6765	0.7941	0.70711
17	-0.2059	1.6765	0.70711
18	0.2647	2.5588	0.70711
19	0.0	1.0	0.0
20	0.4706	1.8824	0.0
21	0.9412	2.7647	0.0
22	1.1471	2.0883	0.70711
23	1.6177	2.9707	0.70711
24	2.0883	3.8530	0.70711
25	1.8236	2.2942	0.0
26	2.2942	3.1766	0.0
27	2.7648	4.0589	0.0
28	2.5	2.5	0.70711
29	2.9706	3.3824	0.70711
30	3.4412	4.2647	0.70711
31	3.6471	3.5883	0.0
32	4.1177	4.4707	0.0
33	4.3236	3.7942	0.70711
34	4.7942	4.6766	0.70711
35	5.0	4.0	0.0

[100] $\Sigma 17a$ 28.07° (041) $\Delta z = 0.0$

$v^{EX} = 0.3850$

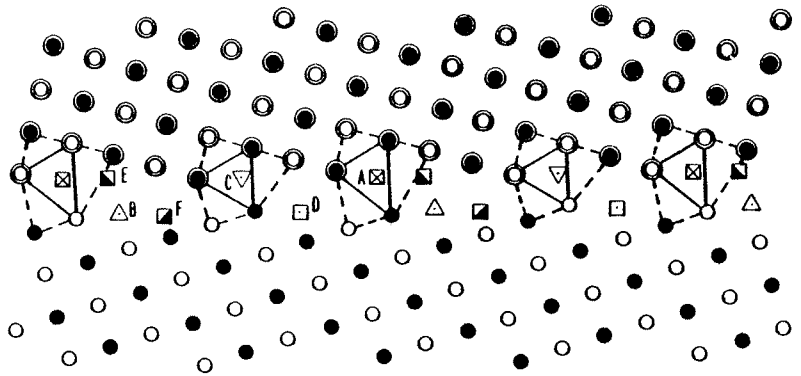
Contacts: 1-19, 3-19, 5-19, 3'-19

Interstitials	x	y	z	d	Touching
A	0.62499	1.37502	0.70711	0.76779	3,5,5',17,20,20',22
B	1.63635	1.36365	0.70711	0.74869	4,6,6',7,22
C	1.25010	1.75000	0.0	0.58121	5,20,22,22',25
(D)	1.91306	2.0	0.70711	0.54207	7,22,25,25',28
(E)	2.29999	1.70000	0.0	0.52316	6,7,7',9,25

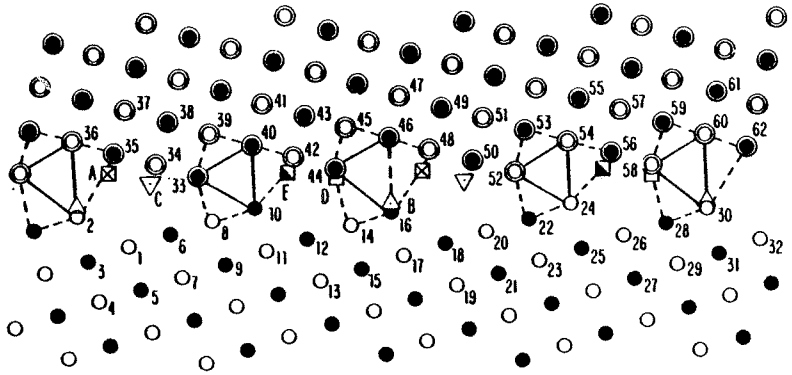
Substitutionals		x	y	z	d	Touching
A	22	1.25006	1.75003	0.70711	1.12139	5,5',20,20',25,25'
B	25	1.90325	2.03225	0.0	1.07355	6,22,22',28,28'
C	5	1.0	1.03337	0.02360	1.00167	3,4,6,19,20

Lattices exactly on the coincidence lattice; CSL sites: 19,28,35

[100] Σ53b 31.89° (072)



⊠ 0.858 △ 0.842 ▽ 0.729 ⊡ 0.696 ◥◣ 0.618 ◢◤ 0.569 Δ Z = 0.044



⊠ 1.130 △ 1.109 ▽ 1.096 ⊡ 1.093 ◥◣ 1.063

[100] Σ53b 31.89° (072) ΔZ = 0.04373

V^{EX} = 0.46567

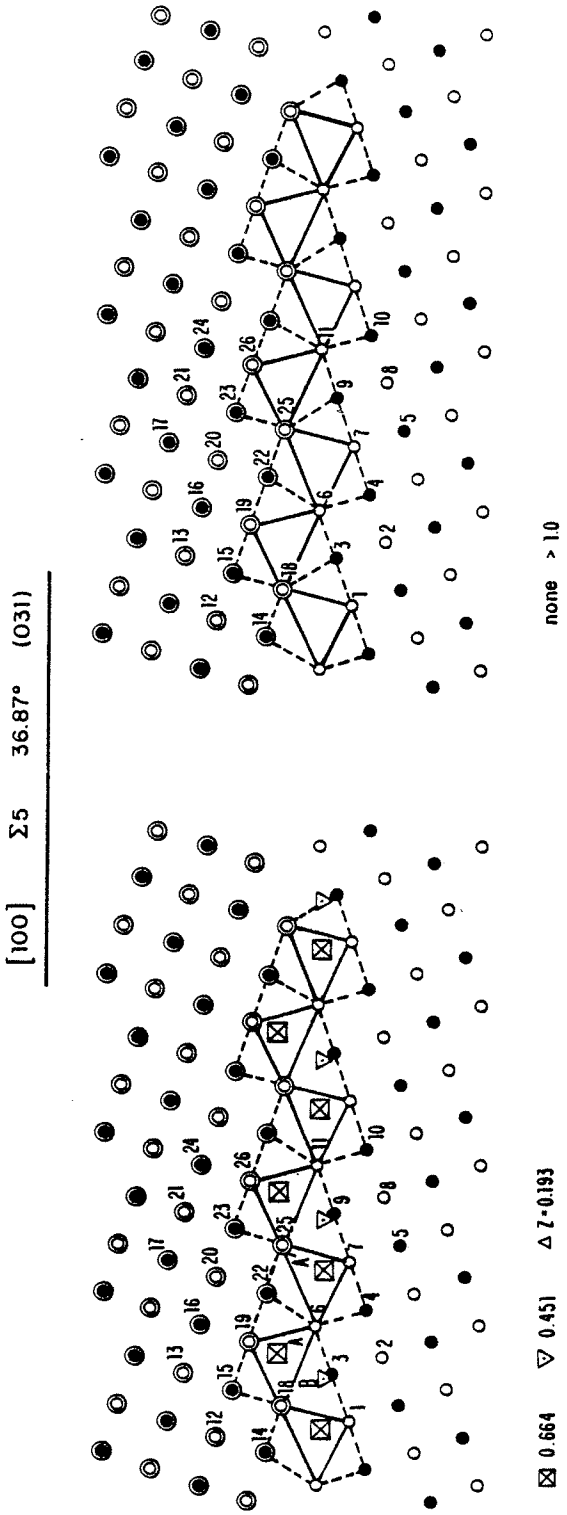
Contacts: 6-33, 10-40 , 8-33.

Interstitials		x	y	z	d	Touching
	A	3.01105	2.92811	0.04302	0.85835	14,16,45,46
	B	-0.41722	0.41721	0.70711	0.84188	1,1',3,6,35
	C	1.08088	1.85956	0.04212	0.72877	8,10,39',40
	D	2.16882	1.83118	0.0000	0.69631	11,12,12',14,42
	E	-0.84728	0.79343	0.04373	0.61831	2,34,35,35',36
	F	0.25972	0.74028	0.0	0.56903	1,6,6',8,34
	G	1.72271	2.22820	-0.66337	0.52550	10,40,42,42',44
	H	2.39968	2.43887	0.04373	0.48985	14,42,44,44'
	I	2.85841	2.14159	0.70711	0.46982	12,14,14',16,44
	J	0.51062	1.51354	0.04374	0.42145	8,33,33',39
	K	0.97073	1.02927	0.70711	0.41663	7,8,8',10,33

Substitutionals		x	y	z	d	Touching
A	35	-0.85347	0.82003	-0.66337	1.12978	2,34,34',36,36'
B	16	3.45450	2.63651	0.70711	1.10875	14,14',18,46
C	34	-0.17678	1.03193	0.04374	1.09576	1,33,33',35,35'
D	44	2.42643	2.57077	-0.66337	1.09267	14,42,42',46
E	42	1.71529	2.26007	0.04373	1.06314	10,40,40',44,44'
F	14	2.88182	2.11818	0.0	1.02774	12,12',16,16',44

[100] Σ53b 31.89° (072) ΔZ = 0.04373

	X	Y	Z		X	Y	Z
1	0.00000	0.00000	0.00000	32	9.00000	5.00000	0.00000
2	-1.00000	-0.00000	0.00000	33	0.44087	1.49729	0.75084
3	-0.50000	-0.50000	0.70711	34	-0.24781	1.33691	0.04373
4	0.00000	-1.00000	0.00000	35	-0.93649	1.17654	-0.66338
5	0.50000	-0.50000	0.70711	36	-1.62517	1.01616	0.04373
6	0.50000	0.50000	0.70711	37	-1.09687	1.86522	0.04373
7	1.00000	0.00000	0.00000	38	-0.40819	2.02559	-0.66338
8	1.00000	1.00000	0.00000	39	0.28049	2.18597	0.04373
9	1.50000	0.50000	0.70711	40	0.96917	2.34635	-0.66338
10	1.50000	1.50000	0.70711	41	0.80879	3.03503	0.04373
11	2.00000	1.00000	0.00000	42	1.65785	2.50673	0.04373
12	2.50000	1.50000	0.70711	43	1.49747	3.19541	-0.66338
13	3.00000	1.00000	0.00000	44	2.34653	2.66710	-0.66338
14	3.00000	2.00000	0.00000	45	2.18615	3.35578	0.04373
15	3.50000	1.50000	0.70711	46	2.87483	3.51616	-0.66338
16	3.50000	2.50000	0.70711	47	2.71445	4.20484	0.04373
17	4.00000	2.00000	0.00000	48	3.56351	3.67654	0.04373
18	4.50000	2.50000	0.70711	49	3.40313	4.36522	-0.66338
19	5.00000	2.00000	0.00000	50	4.25219	3.83692	-0.66338
20	5.00000	3.00000	0.00000	51	4.09181	4.52560	0.04373
21	5.50000	2.50000	0.70711	52	4.94087	3.99729	0.04373
22	5.50000	3.50000	0.70711	53	4.78049	4.68597	-0.66338
23	6.00000	3.00000	0.00000	54	5.46917	4.84635	0.04373
24	6.00000	4.00000	0.00000	55	5.30879	5.53503	-0.66338
25	6.50000	3.50000	0.70711	56	6.15785	5.00673	-0.66338
26	7.00000	4.00000	0.00000	57	5.99747	5.69641	0.04373
27	7.50000	3.50000	0.70711	58	6.84653	5.69541	0.04373
28	7.50000	3.50000	0.70711	59	6.68615	5.16711	0.04373
29	8.00000	4.00000	0.00000	60	7.37483	6.01616	0.04373
30	8.00000	5.00000	0.00000	61	7.21445	6.70484	-0.66338
31	8.50000	4.50000	0.70711	62	8.06351	6.17654	-0.66338



	X	Y	Z
1	0.00000	0.00000	0.70711
2	1.0	0.0	0.70711
3	0.5	0.5	0.0
4	1.5	0.5	0.0
5	2.5	0.5	0.0
6	1.0	1.0	0.70711
7	2.0	1.0	0.70711
8	3.0	1.0	0.70711
9	2.5	1.5	0.0
10	3.5	1.5	0.0
11	3.0	2.0	0.70711
12	-1.02727	1.55455	0.89995
13	-0.42727	2.35455	0.89995
14	-0.92727	0.85455	0.19285
15	-0.32727	1.65455	0.19285
16	0.27273	2.45455	0.19285
17	0.87273	3.25455	0.19285
18	-0.22727	0.95455	0.89995
19	0.37273	1.75455	0.89995
20	0.97273	2.55455	0.89995
21	1.57273	3.35455	0.89995
22	1.07273	1.85455	0.19285
23	1.67273	2.65455	0.19285
24	2.27273	3.45455	0.19285
25	1.77273	1.95455	0.89995
26	2.37273	2.75455	0.89995

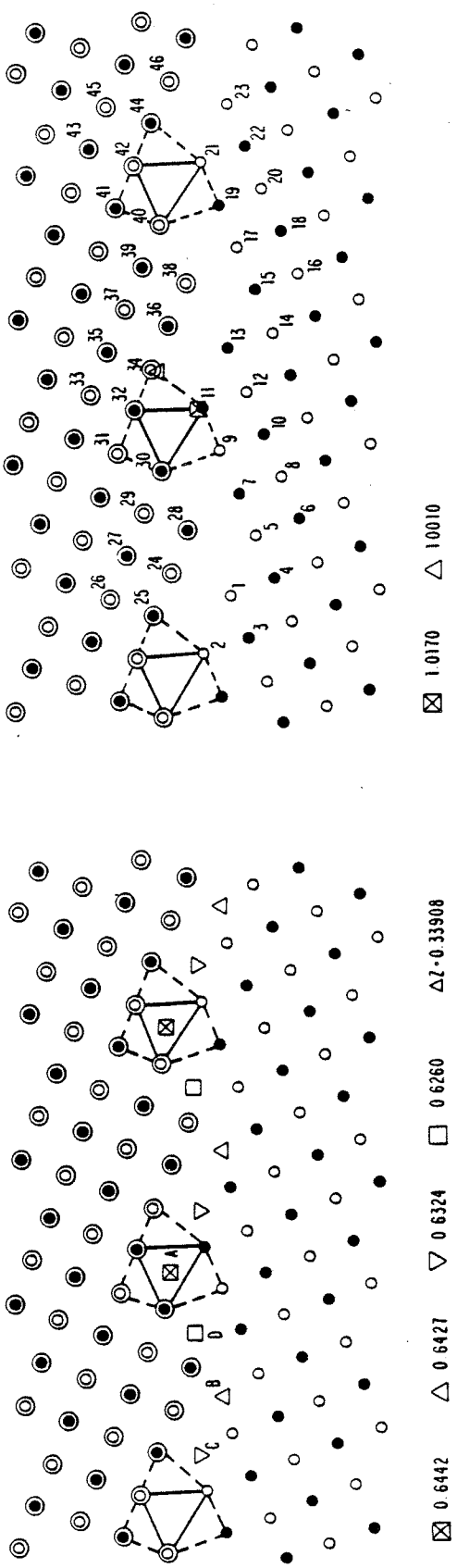
[100] $\Sigma 5$ 36.87° (031) $\Delta z = 0.19285$

$V^{EX} = 0.31945$

Contacts: 1-18, 3-18, 6-19, 6-22'.

Interstitials	x	y	z	d	Touching
A	0.42930	1.30808	0.18570	0.66431	3,6,15,19
A'	1.67677	1.31313	0.00714	0.66431	4,7,22,25
B	0.38462	0.61539	0.70711	0.45138	1,3,3',6,18

Substitutionals none > 1.0



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-1.00000	-0.00000	0.00000
3	-0.50000	-0.50000	0.70711
4	0.50000	-0.50000	0.70711
5	1.00000	-0.00000	0.00000
6	1.50000	-0.50000	0.70711
7	1.50000	0.50000	0.70711
8	2.00000	0.00000	0.00000
9	2.00000	1.00000	0.00000
10	2.50000	0.50000	0.70711
11	2.50000	1.50000	0.70711
12	3.00000	1.00000	0.00000
13	3.50000	1.50000	0.70711
14	4.00000	1.00000	0.00000
15	4.50000	1.50000	0.70711
16	5.00000	1.00000	0.00000
17	5.00000	2.00000	0.00000
18	5.50000	1.50000	0.70711
19	5.50000	2.50000	0.70711
20	6.00000	2.00000	0.00000
21	6.00000	3.00000	0.00000
22	6.50000	2.50000	0.70711
23	7.00000	3.00000	0.00000
24	-0.02687	0.94032	0.33908
25	-0.73578	0.92307	-0.36803
26	-0.75303	1.62997	0.33908
27	-0.04613	1.64721	-0.36803
28	0.67801	0.95756	-0.36803
29	0.66077	1.66445	0.33908
30	1.36766	1.68170	-0.36803
31	1.35042	2.38859	0.33908
32	2.05732	2.40583	-0.36803
33	2.04008	3.11273	0.33908
34	2.76421	2.42308	0.33908
35	2.74697	3.12997	-0.36803
36	3.47111	2.44032	-0.36803
37	3.45387	3.14721	0.33908
38	4.17801	2.45756	0.33908
39	4.16077	3.16446	-0.36803
40	4.86766	3.18170	0.33908
41	4.85042	3.88859	-0.36803
42	5.55732	3.90584	0.33908
43	5.54008	4.61273	-0.36803
44	6.26421	3.92308	-0.36803
45	6.24697	4.62997	0.33908
46	6.97111	3.94032	0.33908

[100] Σ29a 43.60° (052) ΔZ = 0.33908

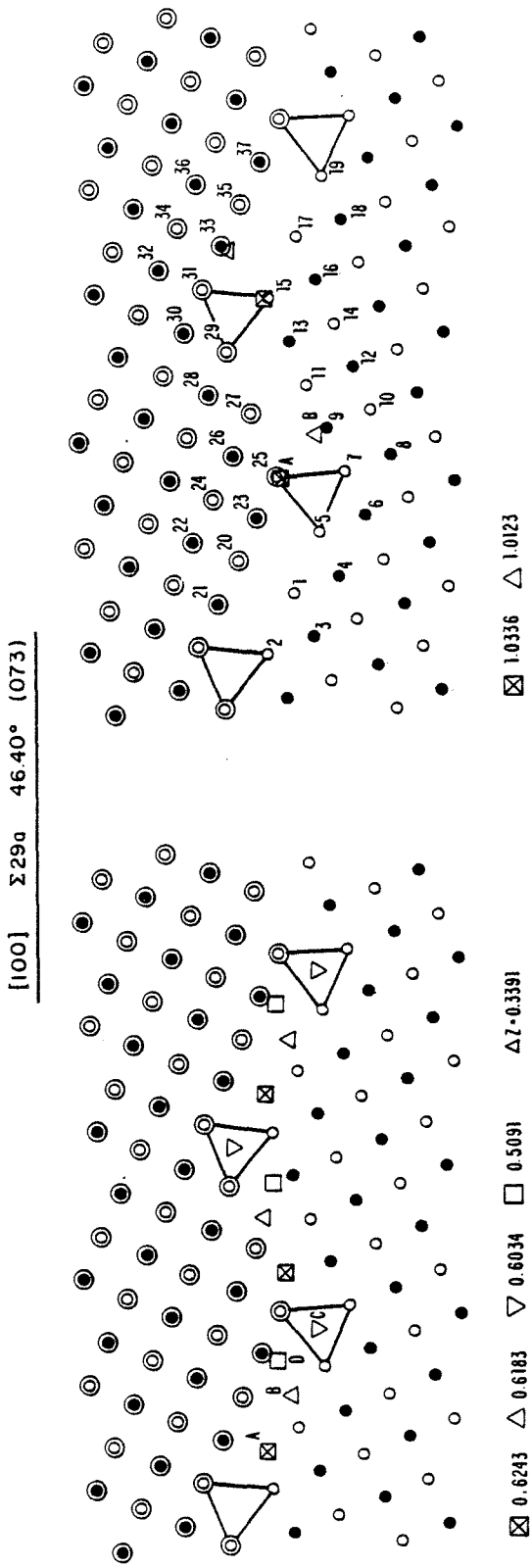
Faceted

V^{EX} = 0.39336

Contacts: 1-24, 7-28, 9-30

Interstitials	x	y	z	d	Touching
A	1.93785	1.82914	0.20558	0.64424	11,30,31,32
B	0.5	0.31030	0.57297	0.64265	1,4,5,28
C	-0.5	0.30442	0.56881	0.63244	1,2,3,25
D	1.22280	1.08928	0.22067	0.62569	7,9,28,29
E	-0.02214	0.66377	-0.36803	0.51858	1,24,24',25,28
F	1.81753	1.18247	0.70711	0.50544	7,9,9',11,30

Substitutionals		x	y	z	d	Touching
A	11	2.49182	1.52453	0.70711	1.01695	9,9',13,34
B	34	2.76498	2.39180	0.33907	1.00097	11,32,32',36,36'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-1.00000	-0.00000	0.00000
3	-0.50000	-0.50000	0.70711
4	0.50000	-0.50000	0.70711
5	1.00000	-0.00000	0.00000
6	1.50000	-0.50000	0.70711
7	2.00000	0.00000	0.00000
8	2.50000	-0.50000	0.70711
9	2.50000	0.50000	0.70711
10	3.00000	0.00000	0.00000
11	3.00000	1.00000	0.00000
12	3.50000	0.50000	0.70711
13	3.50000	1.50000	0.70711
14	4.00000	1.00000	0.00000
15	4.00000	2.00000	0.00000
16	4.50000	1.50000	0.70711
17	5.00000	2.00000	0.00000
18	5.50000	1.50000	0.70711
19	6.00000	2.00000	0.00000
20	0.12715	0.93213	0.33908
21	-0.57975	0.94937	-0.36803
22	0.14439	1.63902	-0.36803
23	0.83405	0.91488	-0.36803
24	0.85129	1.62178	0.33908
25	1.54094	0.89764	0.33908
26	1.55818	1.60454	-0.36803
27	2.26508	1.58730	0.33908
28	2.28232	2.29420	-0.36803
29	2.98922	2.27695	0.33908
30	3.00646	2.98385	-0.36803
31	3.71336	2.96661	0.33908
32	3.73060	3.67351	-0.36803
33	4.42025	2.94937	-0.36803
34	4.43749	3.65627	0.33908
35	5.12715	2.93213	0.33908
36	5.14439	3.63903	-0.36803
37	5.83405	2.91489	-0.36803

[100] $\Sigma 29a$ 46.40° (073) $\Delta Z = 0.33908$

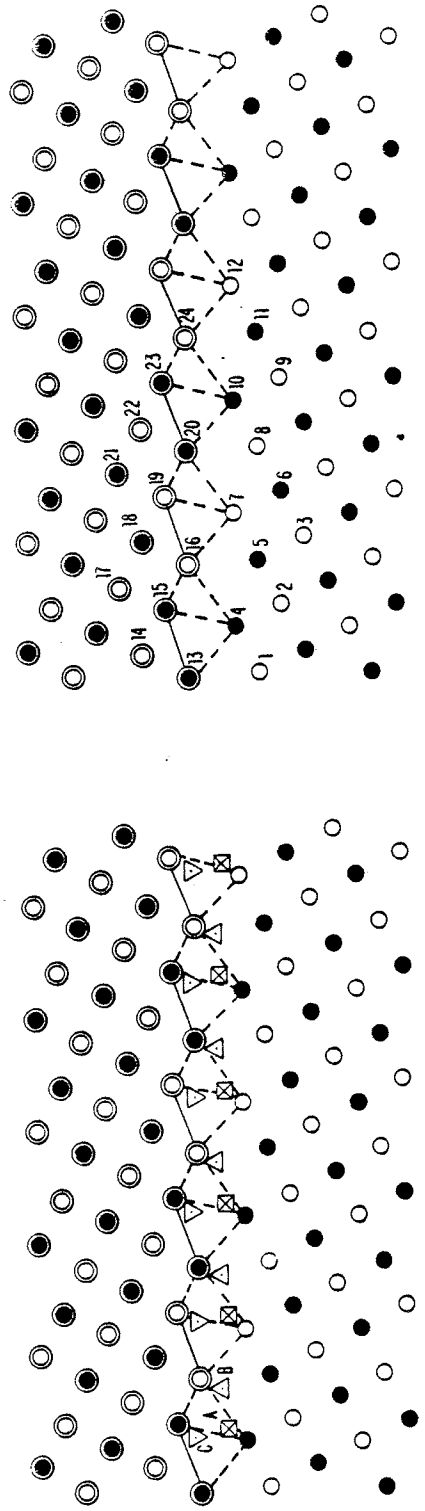
Faceted

$V^{EX} = 0.39735$

Contacts: 1-20, 11-27, 5-23, 13-29

Interstitials	x	y	z	d	Touching
A	-0.5	0.29968	0.56546	0.62426	1,2,3,21
B	0.38791	0.29888	-0.64415	0.61832	1,4,20,23
C	1.5	0.28757	-0.55681	0.60339	5,6,7,25
D	0.82762	0.65165	0.33908	0.50908	5,20,23,25

Substitutionals		x	y	z	d	Touching
A	25	1.56206	0.85270	0.33907	1.03359	7,23,23',27
B	9	2.42137	0.57863	0.70711	1.01233	7,7',11,11',25



	X	Y	Z
1	0.0	0.0	0.0
2	1.0	0.0	0.0
3	2.0	0.0	0.0
4	0.5	0.5	0.70711
5	1.5	0.5	0.70711
6	2.5	0.5	0.70711
7	2.0	1.0	0.0
8	3.0	1.0	0.0
9	4.0	1.0	0.0
10	3.5	1.5	0.70711
11	4.5	1.5	0.70711
12	5.0	2.0	0.0
13	-0.38149	0.84198	1.03273
14	-0.28149	1.54198	0.32562
15	0.41851	1.44198	1.03273
16	1.11851	1.34198	0.32562
17	0.51851	2.14198	0.32562
18	1.21851	2.04198	1.03273
19	1.91851	1.94198	0.32562
20	2.61851	1.84198	1.03273
21	2.01851	2.64198	1.03273
22	2.71851	2.54198	0.32562
23	3.41851	2.44198	1.03273
24	4.11851	2.34198	0.32562

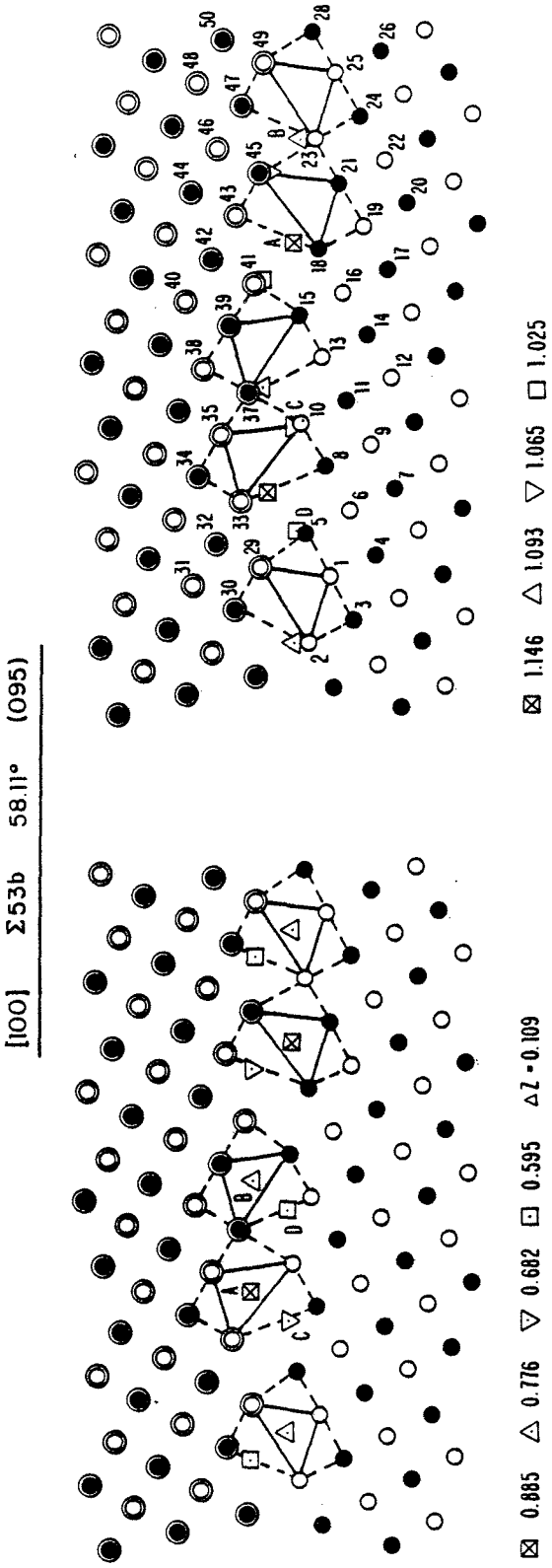
[100] $\Sigma 5$ 53.13° (021) $\Delta z = 0.32562$

$V^{EX} = 0.32210$

Contacts: 1-13, 4-13, 4-15

Interstitials	x	y	z	d	Touching
A	0.65570	0.79984	0.0	0.56734	4,4',15,16
B	1.07674	1.04960	1.03273	0.53262	5,15,16,16'
C	0.37709	1.15203	0.32563	0.53073	4,14,15,15',16
D	1.31181	0.68819	0.0	0.51107	2,5,5',7,16

No Substitutionals



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-1.00000	-0.00000	0.00000
3	-0.50000	-0.50000	0.70711
4	0.50000	-0.50000	0.70711
5	0.50000	0.50000	0.70711
6	1.00000	0.00000	0.00000
7	1.50000	-0.50000	0.70711
8	1.50000	0.50000	0.70711
9	2.00000	0.00000	0.00000
10	2.00000	1.00000	0.00000
11	2.50000	0.50000	0.70711
12	3.00000	0.00000	0.00000
13	3.00000	1.00000	0.00000
14	3.50000	0.50000	0.70711
15	3.50000	1.50000	0.70711
16	4.00000	1.00000	0.00000
17	4.50000	0.50000	0.70711
18	4.50000	1.50000	0.70711
19	5.00000	1.00000	0.00000
20	5.50000	0.50000	0.70711
21	5.50000	1.50000	0.70711
22	6.00000	1.00000	0.00000
23	6.00000	2.00000	0.00000
24	6.50000	1.50000	0.70711
25	7.00000	2.00000	0.00000
26	7.50000	1.50000	0.70711
27	8.00000	2.00000	0.00000
28	7.50000	2.50000	0.70711
29	-0.13839	0.98437	0.10891
30	-0.82707	1.14475	-0.59820
31	-0.66669	1.83343	0.10891
32	0.02199	1.67305	-0.59820
33	0.71067	1.51267	0.10891
34	0.87104	2.20135	-0.59820
35	1.55972	2.04097	0.10891
36	1.72010	2.72965	-0.59820
37	2.24840	1.88060	-0.59820
38	2.40878	2.56928	0.10891
39	3.09746	2.40890	-0.59820
40	3.25784	3.09758	0.10891
41	3.78614	2.24852	0.10891
42	3.94652	2.93720	-0.59820
43	4.63519	2.77682	0.10891
44	4.79557	3.46550	-0.59820
45	5.32387	2.61645	-0.59820
46	5.48425	3.30513	0.10891
47	6.17293	3.14475	-0.59820
48	6.33331	3.83343	0.10891
49	6.86161	2.98437	0.10891
50	7.02199	3.67305	-0.59820
51	7.71067	3.51267	0.10891

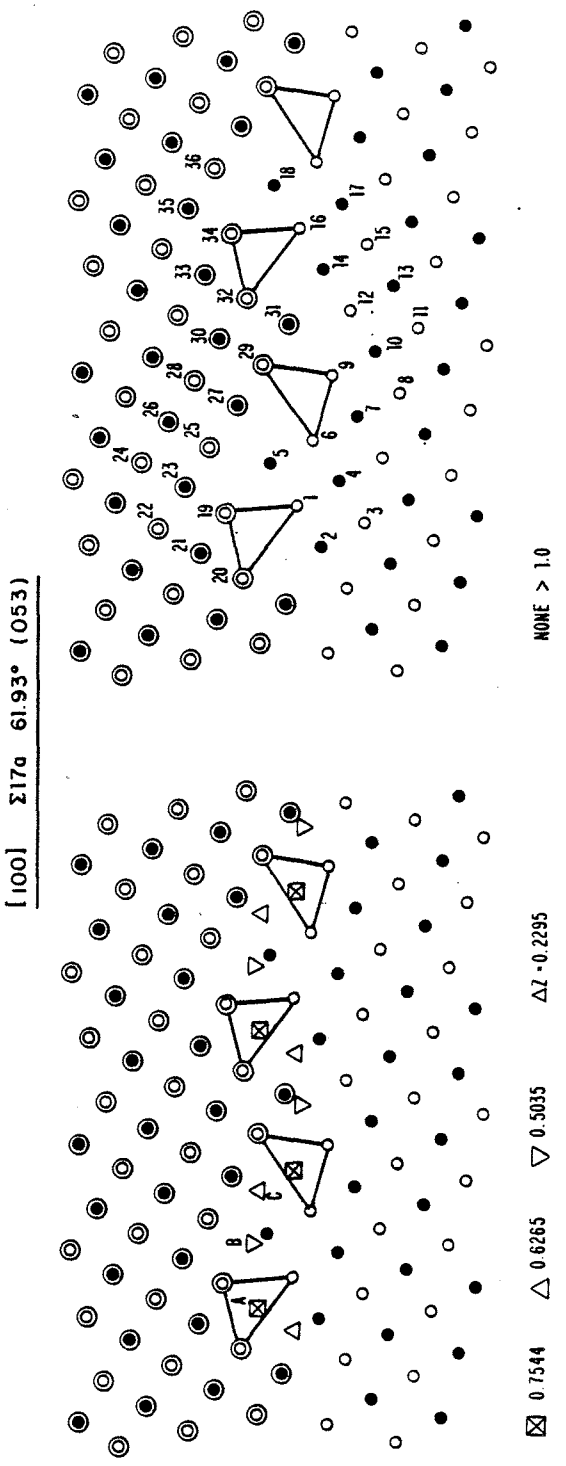
[100] Σ53b 58.11° (095) ΔZ = 0.10891

V^{EX} = 0.48835

Contacts: 1-29, 5-29, 15-39', 15-41.

Interstitials	x	y	z	d	Touching
A	1.41609	1.43255	0.81413	0.88483	8,10,34,35
B	2.97041	1.88137	0.10482	0.77614	13,15,38,39
C	1.17802	0.82198	0.0	0.68207	6,8,8',10,33
D	2.73893	1.26106	0.70711	0.59538	11,13,13',15,37
E	0.64687	1.23871	0.81602	0.52200	5,32,33,33'
F	2.15457	1.15457	0.70711	0.48025	10,10',11,37
G	2.20510	1.69464	0.10891	0.46486	10,35,37,37'
H	3.57443	1.57443	0.0	0.42979	15,15',16,41
I	3.76414	2.15405	0.81602	0.42746	15,39,41,41'

Substitutionals		x	y	z	d	Touching
A	18	4.50000	1.87275	0.81602	1.14551	15,21,41,41'
B	23	5.98079	2.21163	0.10891	1.09325	21,25,45,45'
C	10	1.97127	1.08620	0.0	1.06468	8,8',13,37
D	5	0.50448	0.64963	0.81606	1.02518	6,8,29,29'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.50000	0.70711
3	0.00000	-1.00000	0.00000
4	0.50000	-0.50000	0.70711
5	0.50000	0.50000	0.70711
6	1.00000	0.00000	0.00000
7	1.50000	-0.50000	0.70711
8	2.00000	-1.00000	0.00000
9	2.00000	0.00000	0.00000
10	2.50000	-0.50000	0.70711
11	3.00000	-1.00000	0.00000
12	3.00000	0.00000	0.00000
13	3.50000	-0.50000	0.70711
14	3.50000	0.50000	0.70711
15	4.00000	0.00000	0.00000
16	4.00000	1.00000	0.00000
17	4.50000	0.50000	0.70711
18	4.50000	1.50000	0.70711
19	-0.35187	0.90747	0.22953
20	-1.23422	0.43688	0.22953
21	-1.02834	1.11335	-0.47758
22	-0.82246	1.78983	0.22953
23	-0.14599	1.58394	-0.47758
24	0.05990	2.26041	0.22953
25	0.53048	1.37806	0.22953
26	0.73637	2.05453	-0.47758
27	1.20695	1.17218	-0.47758
28	1.41284	1.84865	0.22953
29	1.88342	0.96630	0.22953
30	2.08931	1.64277	-0.47758
31	2.55990	0.76041	-0.47758
32	2.76578	1.43688	0.22953
33	2.97166	2.11335	-0.47758
34	3.64813	1.90747	0.22953
35	3.85401	2.58394	-0.47758
36	4.53048	2.37806	0.22953

[100] Σ17a 61.93° (053) Δz = 0.22953

Faceted

V^{EX} = 0.40339

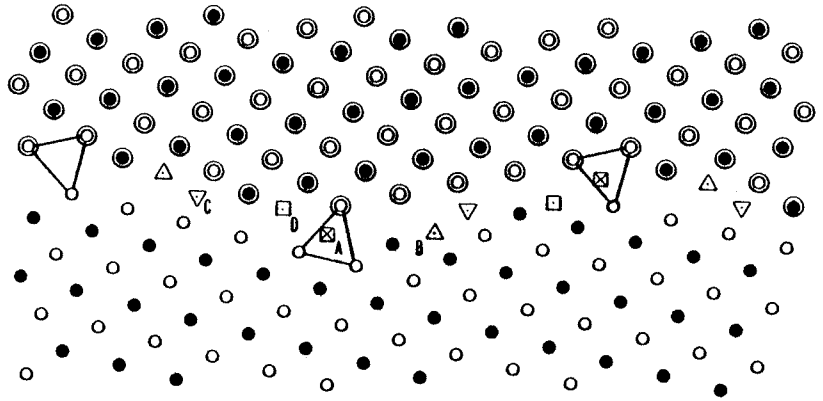
Contacts: 1-19, 9-29, 5-25, 12-31

Interstitials	x	y	z	d	Touching
A	-0.58842	0.35731	0.87052	0.75442	1,2,19,21
B	1.09266	0.77640	1.63784	0.62653	5,6,27,29
C	0.33039	0.69073	0.0	0.50352	5,5',19,25
(D)	-0.12379	0.83946	-0.47776	0.49258	5,19,19',23
(E)	0.47481	1.19515	-0.47756	0.46499	5,23,25,25',27

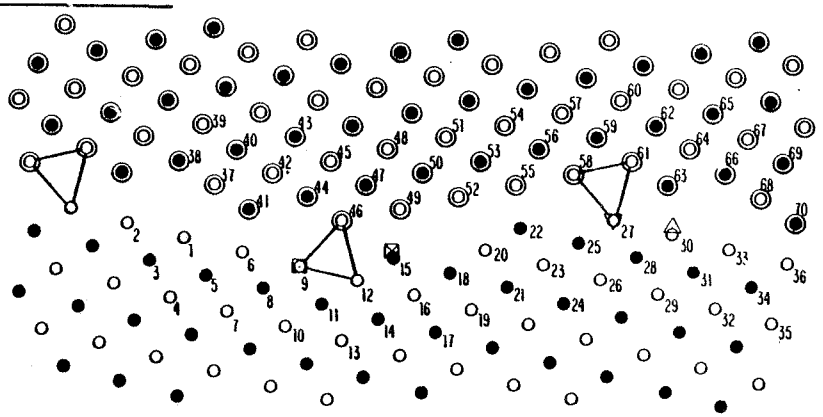
Substitutionals	x	y	z	d	Touching

None > 1.000

[100] Σ85 64.94° (0, 7, 11)



⊠ 0.7724 △ 0.7259 ▽ 0.7248 ⊡ 0.6322 ▵ Z=0.0113



⊠ 1.0517 △ 1.0138 ▽ 1.0093 ⊡ 1.0031

[100] Σ85 64.94° (0,7,11) ΔZ = 0.01133

$V^{EX} = 0.37085$

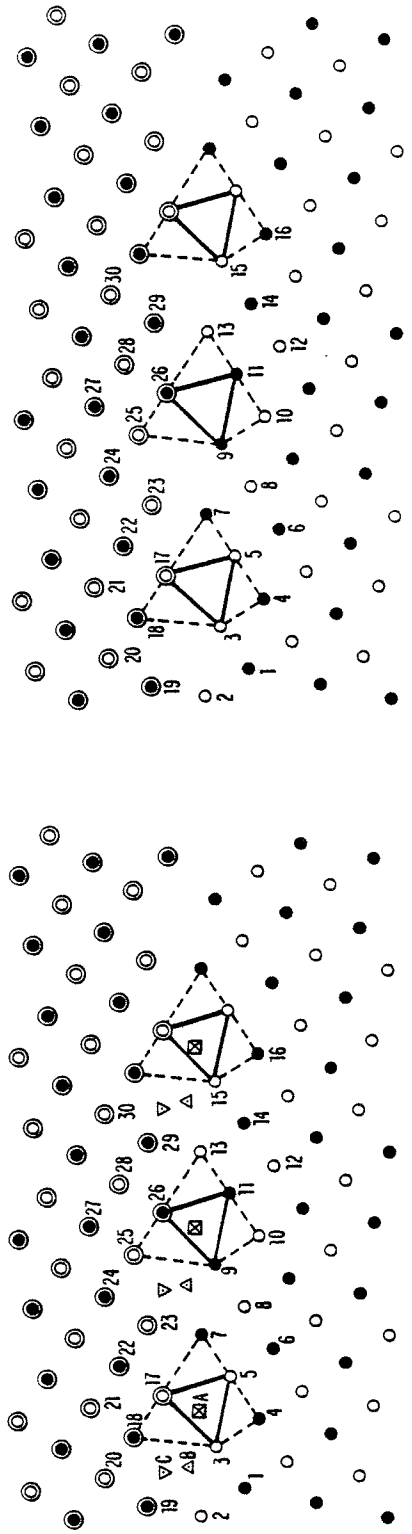
Contacts: 1-37, 20-52, 6-41, 22-55

Interstitials	x	y	z	d	Touching
A	6.66567	2.41661	0.70711	0.77239	27,27',58,59
A	2.39603	0.38000	0.71844	0.77239	9,11,46,46'
B	4.15021	0.84980	0.0	0.72593	16,18,18',30,49
C	0.10276	0.48285	0.70711	0.72476	1,1',37,38
D	1.53367	0.65278	0.14972	0.63218	9,41,42,44
E	1.50003	0.23000	0.89818	0.50892	6,9,41,42
F	3.67395	1.23341	0.71844	0.50768	15,49,50,50'
G	3.39833	0.60167	0.0	0.44315	12,15,15',49
H	0.97786	0.70721	0.01132	0.41529	6,41,41',42
I	1.01199	0.01198	0.70711	0.41462	6,6',8,41

Substitutionals		x	y	z	d	Touching
A	15	3.47658	0.57027	0.70711	1.05166	12,12',18,49
B	30	8.0	2.11706	0.01133	1.01378	27,33,63,63'
C	27	6.99545	2.01365	0.0	1.00928	25,25',30,61
D	9	2.0	0.04561	-0.03224	1.00312	6,8,11,12,46

[100] Σ85 64.94° (0,7,11) ΔZ = 0.01133

	X	Y	Z
1	0.00000	0.00000	0.00000
2	-1.00000	-0.00000	0.00000
3	-0.50000	-0.50000	0.70711
4	0.00000	-1.00000	0.00000
5	0.50000	-0.50000	0.70711
6	1.00000	0.00000	0.00000
7	1.00000	-1.00000	0.00000
8	1.50000	-0.50000	0.70711
9	2.00000	0.00000	0.00000
10	2.00000	-1.00000	0.00000
11	2.50000	-0.50000	0.70711
12	3.00000	0.00000	0.00000
13	3.00000	-1.00000	0.00000
14	3.50000	-0.50000	0.70711
15	3.50000	0.50000	0.70711
16	4.00000	0.00000	0.00000
17	4.50000	-0.50000	0.70711
18	4.50000	0.50000	0.70711
19	5.00000	0.00000	0.00000
20	5.00000	1.00000	0.00000
21	5.50000	0.50000	0.70711
22	5.50000	1.50000	0.70711
23	6.00000	1.00000	0.00000
24	6.50000	0.50000	0.70711
25	6.50000	1.50000	0.70711
26	7.00000	1.00000	0.00000
27	7.00000	2.00000	0.00000
28	7.50000	1.50000	0.70711
29	8.00000	1.00000	0.00000
30	8.00000	2.00000	0.00000
31	8.50000	1.50000	0.70711
32	9.00000	1.00000	0.00000
33	9.00000	2.00000	0.00000
34	9.50000	1.50000	0.70711
35	10.00000	1.00000	0.00000
36	10.00000	2.00000	0.00000
37	0.28715	0.95782	0.01133
38	-0.37756	1.19900	-0.69578
39	-0.13638	1.86370	0.01133
40	0.52833	1.62253	-0.69578
41	0.95186	0.71664	-0.69578
42	1.19303	1.38135	0.01133
43	1.43421	2.04605	-0.69578
44	1.85774	1.14017	-0.69578
45	2.09891	1.80488	0.01133
46	2.52244	0.89900	0.01133
47	2.76362	1.56370	-0.69578
48	3.00480	2.22841	0.01133
49	3.42833	1.32253	0.01133
50	3.66950	1.98723	-0.69578
51	3.91068	2.65194	0.01133
52	4.33421	1.74606	0.01133
53	4.57539	2.41076	-0.69578
54	4.81656	3.07547	0.01133
55	5.24009	2.16959	0.01133
56	5.48127	2.83429	-0.69578
57	5.72244	3.49900	0.01133
58	6.14597	2.59311	0.01133
59	6.38715	3.25782	-0.69578
60	6.62833	3.92253	0.01133
61	7.05186	3.01664	0.01133
62	7.29303	3.68135	-0.69578
63	7.71656	2.77547	-0.69578
64	7.95774	3.44017	0.01133
65	8.19892	4.10488	-0.69578
66	8.62245	3.19900	-0.69578
67	8.86362	3.86370	0.01133
68	9.28715	2.95782	0.01133
69	9.52833	3.62253	-0.69578
70	9.95186	2.71665	-0.69578



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	0.50000	0.70711
3	0.50000	0.50000	0.70711
4	1.00000	0.00000	0.00000
5	1.50000	0.50000	0.70711
6	2.00000	0.00000	0.00000
7	2.00000	1.00000	0.00000
8	2.50000	0.50000	0.70711
9	3.00000	1.00000	0.00000
10	3.50000	0.50000	0.70711
11	4.00000	1.00000	0.00000
12	4.50000	0.50000	0.70711
13	4.50000	1.50000	0.70711
14	5.00000	1.00000	0.00000
15	5.50000	1.50000	0.70711
16	6.00000	1.00000	0.00000
17	1.00000	1.36462	0.65782
18	0.34615	1.63385	-0.04929
19	-0.57692	1.24923	-0.04929
20	-0.30769	1.90308	0.65782
21	0.61538	2.28769	0.65782
22	1.26923	2.01846	-0.04929
23	1.92308	1.74923	0.65782
24	2.19231	2.40308	-0.04929
25	2.84615	2.13385	0.65782
26	3.50000	1.86462	-0.04929
27	3.11538	2.78769	-0.04929
28	3.76923	2.51846	0.65782
29	4.42308	2.24923	-0.04929
30	4.69231	2.90308	0.65782

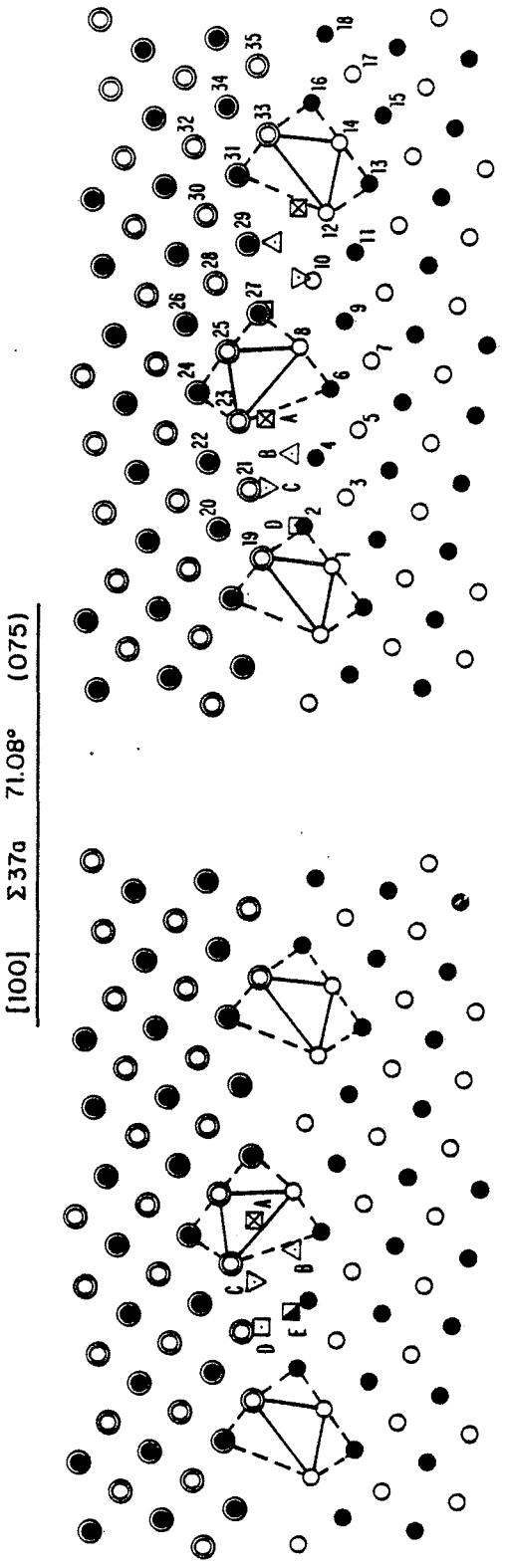
[100] Σ13a 67.38° (023) Δz = -0.04929

V^{EX} = 0.40132

Contacts: 3-17,5-17,7-23

Interstitials	x	y	z	d	Touching
A	0.93606	0.86495	-0.04889	0.73963	3,4,17,17'
B	0.14148	0.82508	0.02365	0.67490	1,3,18,19
C	0.0	1.14982	0.78556	0.64730	2,3,19,20

Substitutionals none > 1.0



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	0.50000	0.70711
3	1.00000	0.00000	0.00000
4	1.50000	0.50000	0.70711
5	2.00000	0.00000	0.00000
6	2.50000	0.50000	0.70711
7	3.00000	0.00000	0.00000
8	3.00000	1.00000	0.00000
9	3.50000	0.50000	0.70711
10	4.00000	1.00000	0.00000
11	4.50000	0.50000	0.70711
12	5.00000	1.00000	0.00000
13	5.50000	0.50000	0.70711
14	6.00000	1.00000	0.00000
15	6.50000	0.50000	0.70711
16	6.50000	1.50000	0.70711
17	7.00000	1.00000	0.00000
18	7.50000	1.50000	0.70711
19	-0.08246	0.99465	0.06209
20	0.22835	1.62979	0.76920
21	0.86349	1.31897	0.06209
22	1.17430	1.95411	0.76920
23	1.80943	1.64330	0.06209
24	2.12024	2.27843	0.76920
25	2.75538	1.96762	0.06209
26	3.06619	2.60276	0.76920
27	3.39051	1.65681	0.76920
28	3.70132	2.29195	0.06209
29	4.33646	1.98114	0.76920
30	4.64727	2.61627	0.06209
31	5.28241	2.30546	0.76920
32	5.59322	2.94060	0.06209
33	5.91754	1.99465	0.06209
34	6.22835	2.62979	0.76920
35	6.86349	2.31898	0.06209

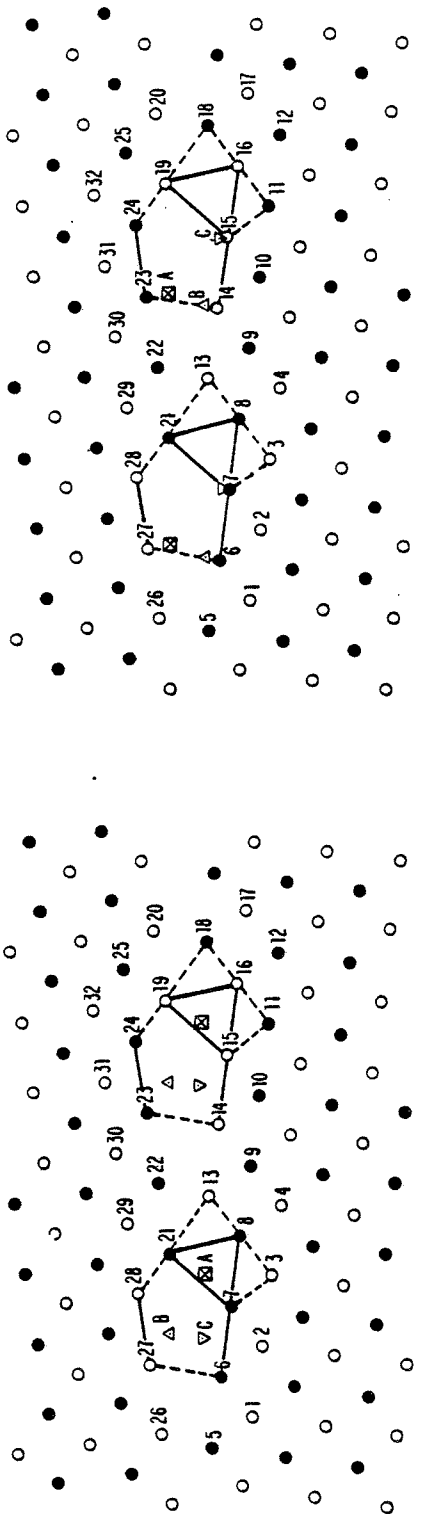
[100] Σ37a 71.08° (075) $\Delta z = 0.06209$

$$v^{EX} = 0.47063$$

Contacts: 1-19, 8-25, 2-19

Interstitials	x	y	z	d	Touching
A	2.48846	1.42628	0.76740	0.85662	6,8,24,25
B	2.14886	0.85114	0.0	0.72811	5,6,6',8,23
C	1.63807	1.29313	0.76920	0.61490	4,22,23,23'
D	1.0	1.07114	0.76920	0.52322	2,4,21,21'
(E)	1.30085	0.69915	0.0	0.52226	3,4,4',21
(F)	0.62969	0.62968	0.0	0.46101	2,2',3,21

Substitutionals		x	y	z	d	Touching
A	23	1.94315	1.25330	-0.05850	1.17671	4,8,21,25
B	4	1.5	0.84922	0.76920	1.12208	2,6,21,21'
C	21	0.93730	1.10368	0.0	1.05490	2,2',17,23
D	2	0.50163	0.58619	0.76922	1.00799	3,4,19,19'



	X	Y	Z
1	0.00000	0.00000	0.70711
2	1.00000	0.00000	0.70711
3	2.00000	0.00000	0.70711
4	3.00000	0.00000	0.70711
5	-0.50000	0.50000	0.00000
6	0.50000	0.50000	0.00000
7	1.50000	0.50000	0.00000
8	2.50000	0.50000	0.00000
9	3.50000	0.50000	0.00000
10	4.50000	0.50000	0.00000
11	5.50000	0.50000	0.00000
12	6.50000	0.50000	0.00000
13	3.00000	1.00000	0.70711
14	4.00000	1.00000	0.70711
15	5.00000	1.00000	0.70711
16	6.00000	1.00000	0.70711
17	7.00000	1.00000	0.70711
18	6.50000	1.50000	0.00000
19	5.61539	1.92308	0.70711
20	6.57539	2.20308	0.70711
21	2.11539	1.42308	0.00000
22	3.07539	1.70308	0.00000
23	4.03539	1.98308	0.00000
24	4.99539	2.26308	0.00000
25	5.95539	2.54308	0.00000
26	-0.42461	1.20308	0.70711
27	0.53539	1.48308	0.70711
28	1.49539	1.76308	0.70711
29	2.45539	2.04308	0.70711
30	3.41539	2.32308	0.70711
31	4.37539	2.60308	0.70711
32	5.33539	2.88308	0.70711

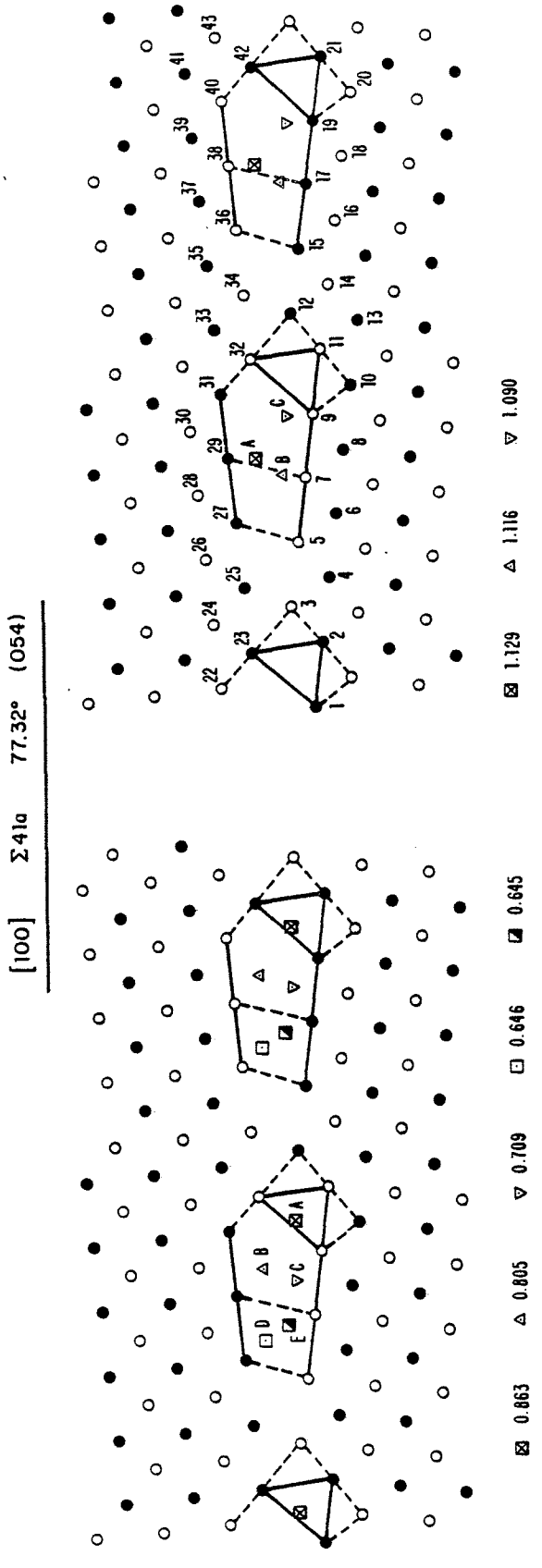
[100] Σ25a 73.74° (043) $\Delta z = 0$

$v^{EX} = 0.45180$

Contacts: 8-21, 13-22, 13-22'

Interstitials	x	y	z	d	Touching
A	1.9	0.9	0.70711	0.81108	3,7,7',21,21'
B	1.0	1.22841	0.0	0.76701	6,7,27,27',unnumbered repeats at 14,15,23,23',31
C	1.0	0.81432	0.83841	0.64967	2,6,7,27
(D)	3.72650	1.25641	0.01209	0.57938	9,14,22,23
(E)	3.5	1.56977	0.61983	0.52611	13,14,23,31

Substitutionals		x	y	z	d	Touching
A	23	4.10551	1.74268	0.0	1.06175	14,14',22,24
B	14	4.0	1.23787	0.70711	1.05580	13,15,23,23'
C	15	5.0	1.12501	0.61872	1.02330	10,11,14,16,19



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	1.50000	0.50000	0.70711
4	2.00000	0.00000	0.00000
5	2.50000	0.50000	0.70711
6	3.00000	0.00000	0.00000
7	3.50000	0.50000	0.70711
8	4.00000	0.00000	0.00000
9	4.50000	0.50000	0.70711
10	5.00000	0.00000	0.00000
11	5.50000	0.50000	0.70711
12	6.00000	1.00000	0.00000
13	6.00000	0.00000	0.00000
14	6.50000	0.50000	0.70711
15	7.00000	1.00000	0.00000
16	7.50000	0.50000	0.70711
17	8.00000	1.00000	0.00000
18	8.50000	0.50000	0.70711
19	9.00000	1.00000	0.00000
20	9.50000	0.50000	0.70711
21	10.00000	1.00000	0.00000
22	0.12244	1.33805	0.70711
23	0.72000	0.96000	0.00000
24	1.09805	1.55756	0.70711
25	1.69561	1.17951	0.00000
26	2.07366	1.77707	0.70711
27	2.67122	1.39903	0.00000
28	3.04927	1.99659	0.70711
29	3.64683	1.61854	0.00000
30	4.02488	2.21610	0.70711
31	4.62244	1.83805	0.00000
32	5.22000	1.46000	0.70711
33	5.59805	2.05756	0.00000
34	6.19561	1.67951	0.70711
35	6.57366	2.27708	0.00000
36	7.17122	1.89903	0.70711
37	7.54927	2.49659	0.00000
38	8.14683	2.11854	0.70711
39	8.52488	2.71610	0.00000
40	9.12244	2.33805	0.70711
41	9.50049	2.93561	0.00000
42	9.72000	1.96000	0.00000
43	10.09805	2.55756	0.70711

[100] $\Sigma 41a$ 77.32° (054) $\Delta Z = 0$

$V^{EX} = 0.48590$

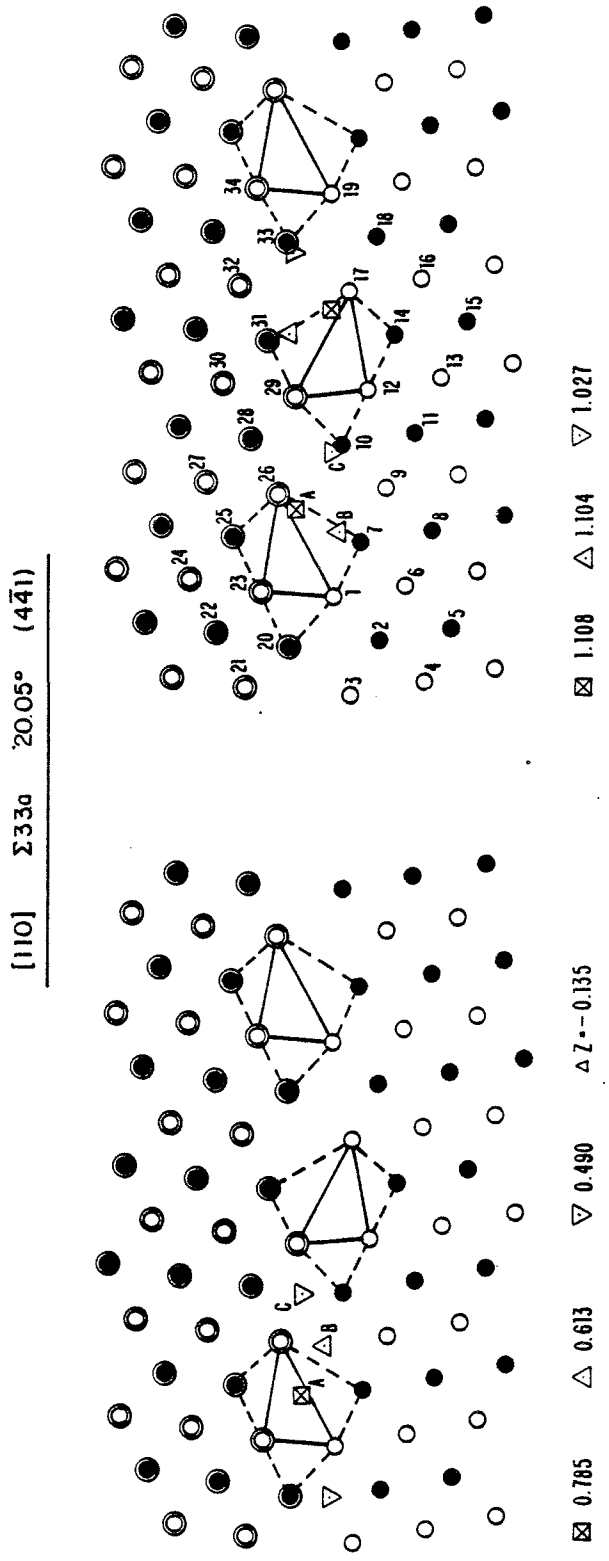
Contacts: 2-23, 3-25, 3-25'.

Interstitials	x	y	z	d	Touching
A	4.92857	0.92857	0.0	0.86263	9,9',10,32,32'
B	4.12063	1.31879	0.70711	0.80481	9,29,29',30
C	4.0	0.84780	0.10726	0.70921	7,8,9,29
D	3.02725	1.17379	0.70711	0.64619	7,27,27',28
E	3.30245	0.87143	0.0	0.64550	7,7',27,29
F	2.31065	0.72381	0.0	0.53093	5,5',25,27
G	2.0	1.04278	0.6	0.47897	3,5,25,26

Substitutionals		x	y	z	d	Touching
A	29	3.72691	1.26263	0.0	1.12893	7,7',27,31
B	7	3.5	0.84540	0.70711	1.11594	5,9,29,29'
C	9	4.41333	0.88445	0.37398	1.09089	7,8,31,32
D	27	2.71535	1.20288	0.0	1.04002	5,5',25,29
E	5	2.5	0.68774	0.70711	1.03494	3,7,27,27'
F	31	4.55874	1.20595	0.0	1.00181	9,9',29,32,32'

5.2 DENSEST [110] BOUNDARIES

Listed in order of increasing angle



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	-0.70711	0.50000
3	0.00000	-1.41421	0.00000
4	1.00000	-1.41421	0.00000
5	1.50000	-0.70711	0.50000
6	1.00000	-0.00000	0.00000
7	0.50000	0.70711	0.50000
8	1.50000	0.70711	0.50000
9	1.00000	1.41421	0.00000
10	0.50000	2.12132	0.50000
11	1.50000	2.12132	0.50000
12	1.00000	2.82843	0.00000
13	2.00000	2.82843	0.00000
14	1.50000	3.53553	0.50000
15	2.50000	3.53553	0.50000
16	2.00000	4.24264	0.00000
17	1.00000	4.24264	0.00000
18	1.50000	4.94975	0.50000
19	1.00000	5.65685	0.00000
20	-0.72957	-0.57814	0.36536
21	-1.44169	-1.07097	0.86536
22	-1.66896	-0.23530	0.36536
23	-0.95684	0.25753	0.86536
24	-1.89624	0.60037	0.86536
25	-1.18412	1.09321	0.36536
26	-0.47199	1.58604	0.86536
27	-1.41139	1.92888	0.86536
28	-0.69927	2.42171	0.36536
29	0.01285	2.91454	0.86536
30	-0.92654	3.25738	0.86536
31	-0.21442	3.75021	0.36536
32	-0.44169	4.58589	0.86536
33	0.27043	5.07872	0.36536
34	0.04315	5.91439	0.86536

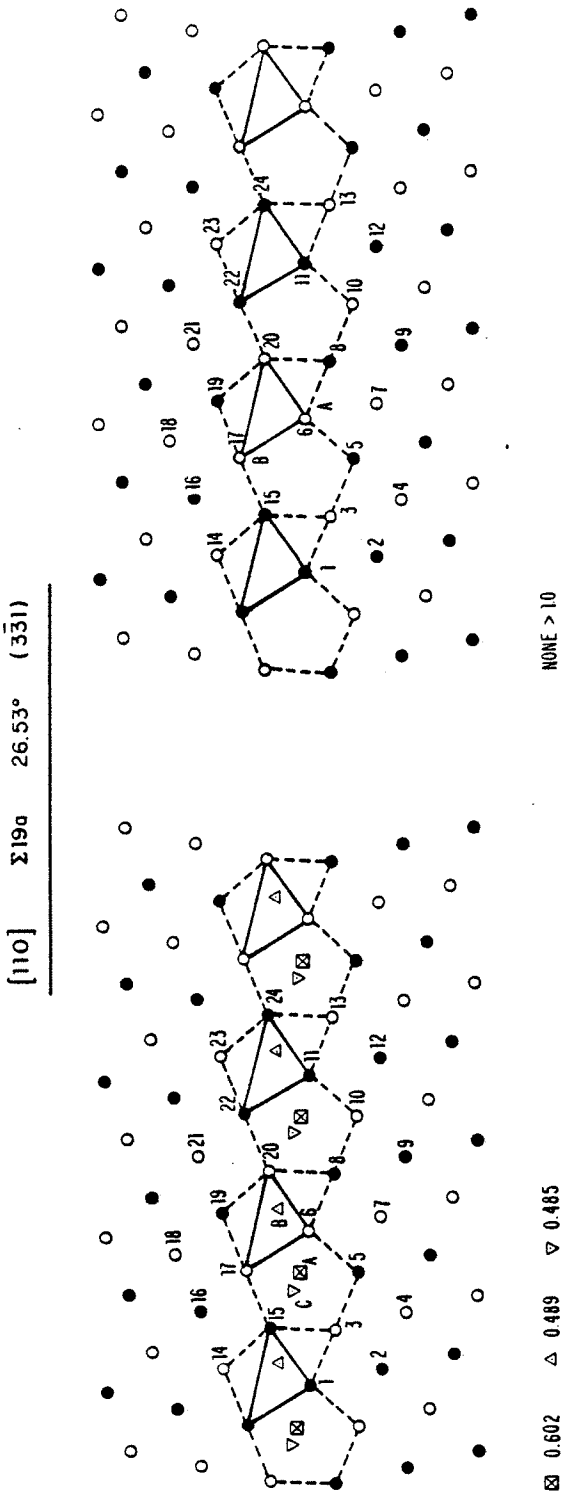
[110] $\Sigma 33a$ 20.05° $(4\bar{4}1)$ $\Delta Z = -0.13464$

$V^{EX} = 0.41711$

Contacts: 1-20, 1-23, 10-29, 12-29.

Interstitials	x	y	z	d	Touching
A	-0.35276	0.78965	0.25032	0.78481	7,23,25,26
B	0.13674	1.41422	0.36536	0.61255	7,10,26,26'
C	-0.19243	-0.70711	-0.13464	0.49017	1,3,20,20'

Substitutionals		x	y	z	d	Touching
A	26	-0.28226	1.31188	-0.13464	1.10823	7,25,25',26',26"
B	7	0.23305	0.89587	0.5	1.10418	1,1',7',7",9,9',26
C	10	0.36495	2.02582	0.5	1.02718	9,9',10',10",26



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	0.50000	0.70711	0.50000
4	1.50000	0.70711	0.50000
5	1.00000	1.41421	0.00000
6	0.50000	2.12132	0.50000
7	1.50000	2.12132	0.50000
8	1.00000	2.82843	0.00000
9	2.00000	2.82843	0.00000
10	1.50000	3.53553	0.50000
11	1.00000	4.24264	0.00000
12	2.00000	4.24264	0.00000
13	1.50000	4.94975	0.50000
14	-1.08763	0.56277	0.50000
15	-0.32447	0.97215	0.00000
16	-1.21921	1.41874	0.00000
17	-0.45605	1.82812	0.50000
18	-1.35079	2.27471	0.50000
19	-0.58763	2.68409	0.00000
20	-0.17553	3.09347	0.50000
21	-0.71921	3.54006	0.50000
22	0.04395	3.94944	0.00000
23	-0.08763	4.80541	0.50000
24	0.67553	5.21479	0.00000

[110] Σ19a 26.53° $(3\bar{3}1)$ $\Delta Z = 0.$

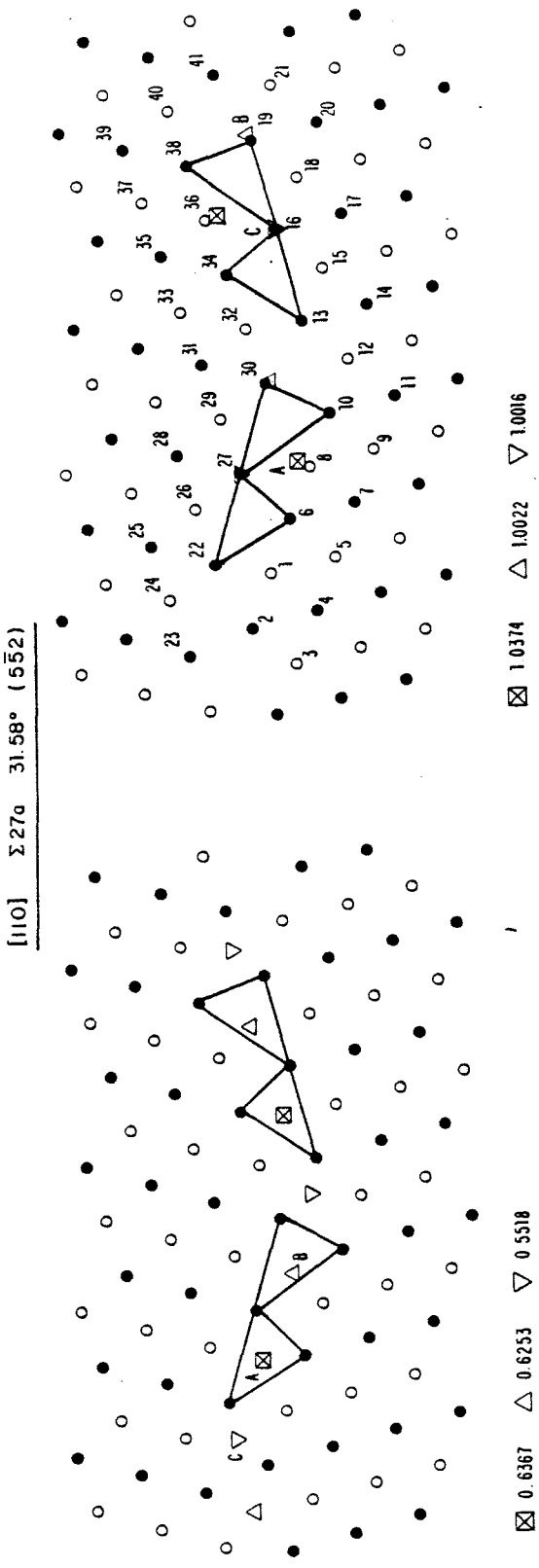
$V^{EX} = 0.24066$

Contacts: 3-15, 3-15', 6-17

Interstitials	x	y	z	d	Touching
A	0.21359	1.56524	0.0	0.60157	5,6,6',15
B	0.14347	2.54254	0.0	0.48936	6,6',19,20,20'
C	0.09328	1.32843	0.5	0.48519	3,15,15',17
D	-0.12471	2.45304	0.48263	0.41507	6,17,19,20

Substitutionals	x	y	z	d	Touching

None > 1.0000



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.70711	0.50000
3	0.00000	-1.41421	0.00000
4	0.50000	-0.70711	0.50000
5	1.00000	0.00000	0.00000
6	0.50000	0.70711	0.50000
7	1.50000	0.70711	0.50000
8	1.00000	1.41421	0.00000
9	2.00000	1.41421	0.00000
10	1.50000	2.12132	0.50000
11	2.50000	2.12132	0.50000
12	2.00000	2.82843	0.00000
13	1.50000	3.53553	0.50000
14	2.50000	3.53553	0.50000
15	2.00000	4.24264	0.00000
16	1.50000	4.94975	0.50000
17	2.50000	4.94975	0.50000
18	2.00000	5.65685	0.00000
19	1.50000	6.36396	0.50000
20	2.50000	6.36396	0.50000
21	2.00000	7.07107	0.00000
22	-0.78594	0.36372	0.50000
23	-1.52669	-0.84098	0.50000
24	-1.58224	0.02326	0.00000
25	-1.63780	0.88750	0.50000
26	-0.84150	1.22796	0.00000
27	-0.04520	1.56842	0.50000
28	-0.89706	2.09220	0.50000
29	-0.10076	2.43266	0.00000
30	0.69554	2.77312	0.50000
31	-0.15632	3.29690	0.50000
32	0.63998	3.63736	0.00000
33	-0.21187	4.16114	0.00000
34	0.58442	4.50160	0.50000
35	-0.26743	5.02539	0.50000
36	0.52887	5.36584	0.00000
37	-0.32298	5.88963	0.00000
38	0.47331	6.23009	0.50000
39	-0.37854	6.75387	0.50000
40	0.41776	7.09433	0.00000
41	1.21405	7.43479	0.50000

[110] $\Sigma 27a$ 31.58° $(5\bar{5}2)$ $\Delta z = 0.$

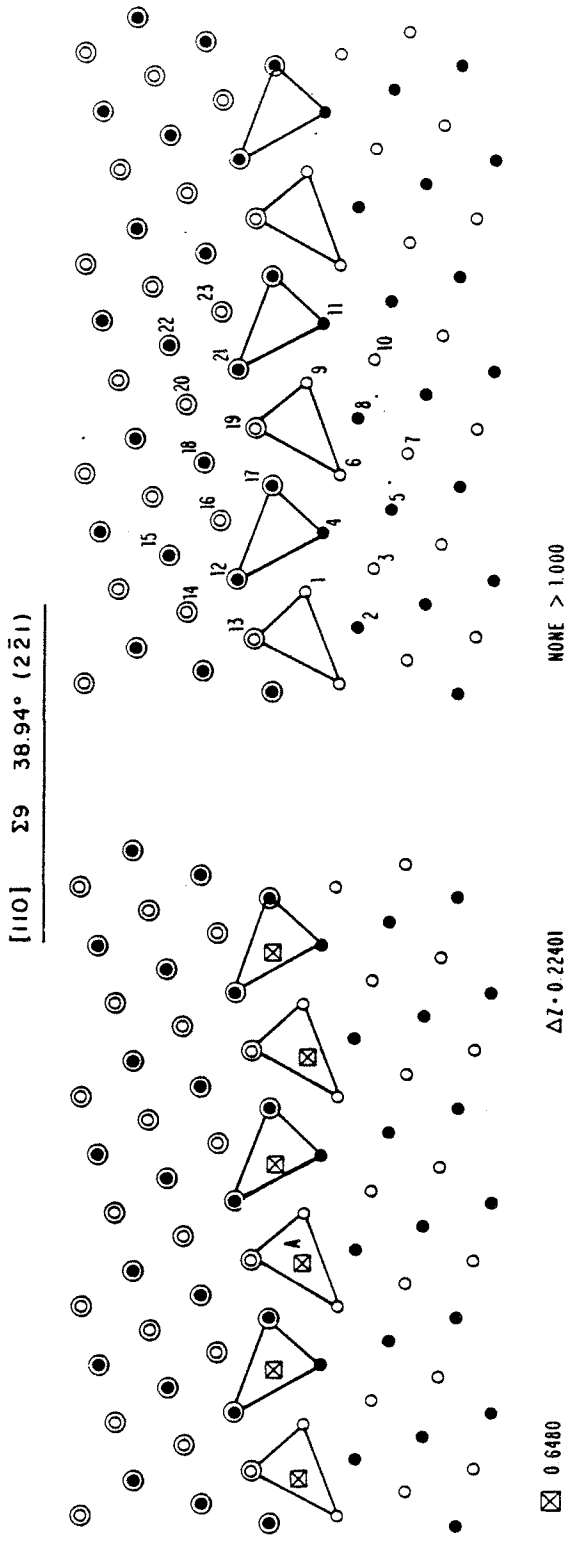
Faceted

$V^{EX} = 0.31195$

Contacts: 1-22, 1-22', 13-32, 13-32'

Interstitials	x	y	z	d	Touching
A	-0.14020	0.80624	0.0	0.63668	1,6,6',26
B	0.66630	1.96102	0.5	0.62525	8,8',27,30
C	-0.84763	-0.22631	0.0	0.55179	2,2',22,22',24
D	0.31370	1.19239	0.0	0.44251	6,6',8,27,27'

Substitutionals		x	y	z	d	Touching
A	8	0.84136	1.52639	0.0	1.03740	6,6',8',8'',10,10',27,27'
B	19	1.46137	6.39128	0.5	1.00224	19',19'',21,21',38
C	16	1.46733	4.97285	0.5	1.00160	16',16'',18,18',34
D	10	1.47155	2.14144	0.5	1.00121	8,8',10',10'',12,12',30
E	6	0.48306	0.71908	0.5	1.00043	1,1',6',6'',8,8',27



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	-0.70711	0.50000
3	1.00000	0.00000	0.00000
4	0.50000	0.70711	0.50000
5	1.50000	0.70711	0.50000
6	1.00000	1.41421	0.00000
7	2.00000	1.41421	0.00000
8	1.50000	2.12132	0.50000
9	1.00000	2.82843	0.00000
10	2.00000	2.82843	0.00000
11	1.50000	3.53553	0.50000
12	-0.83691	0.47267	0.27599
13	-0.89246	-0.39157	0.77599
14	-1.67024	0.23697	0.77599
15	-1.61468	1.10121	0.27599
16	-0.78135	1.33691	0.77599
17	0.05198	1.57261	0.27599
18	-0.72580	2.20115	0.27599
19	0.10754	2.43685	0.77599
20	-0.67024	3.06539	0.77599
21	0.16309	3.30110	0.27599
22	-0.61469	3.92964	0.27599
23	0.21865	4.16534	0.77599

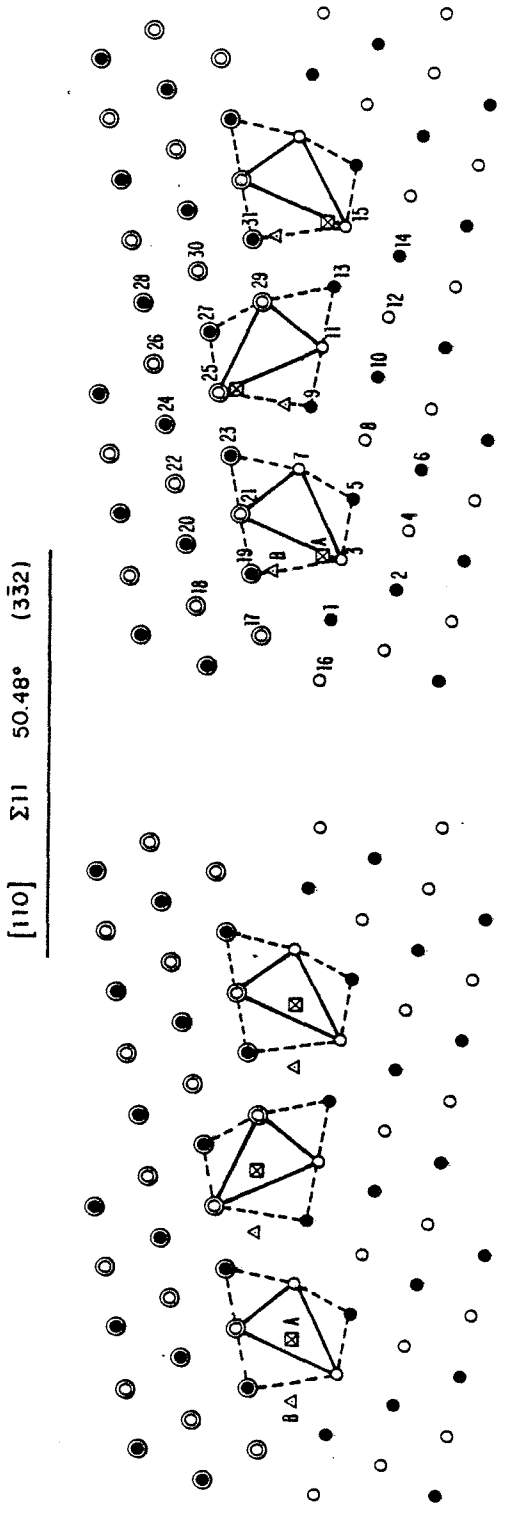
[110] Σ9 38.94° $(2\bar{2}1)$ $\Delta z = 0.22401$

$V^{EX} = 0.26882$

Contacts: 1-12, 1-13, 4-17, 6-17

Interstitials	x	y	z	d	Touching
A	-.70086	2.12132	0.29914	0.64800	6,8,9,19

Substitutionals	x	y	z	d	Touching
None > 1.000					



	X	Y	Z
1	0.50000	0.70711	0.00000
2	1.50000	0.70711	0.00000
3	1.00000	1.41421	0.50000
4	2.00000	1.41421	0.50000
5	1.50000	2.12132	0.00000
6	2.50000	2.12132	0.00000
7	1.00000	2.82842	0.50000
8	2.00000	2.82842	0.50000
9	1.50000	3.53550	0.00000
10	2.50000	3.53550	0.00000
11	2.00000	4.24260	0.50000
12	3.00000	4.24260	0.50000
13	2.50000	4.94970	0.00000
14	3.50000	4.94970	0.00000
15	3.00000	5.65690	0.50000
16	0.00000	0.00000	0.50000
17	-0.41145	0.90081	0.63690
18	-1.04775	1.67221	0.63690
19	-0.18415	1.73651	0.13690
20	-0.82045	2.50791	0.13690
21	0.04315	2.57211	0.63690
22	-0.59315	3.34371	0.63690
23	0.27045	3.40801	0.13690
24	-0.36585	4.17941	0.13690
25	0.49775	4.24381	0.63690
26	-0.13855	5.01521	0.63690
27	0.72505	5.07951	0.13690
28	0.08875	5.85091	0.13690
29	1.58875	5.14381	0.63690
30	0.95245	5.91521	0.63690
31	1.81605	5.97951	0.13690

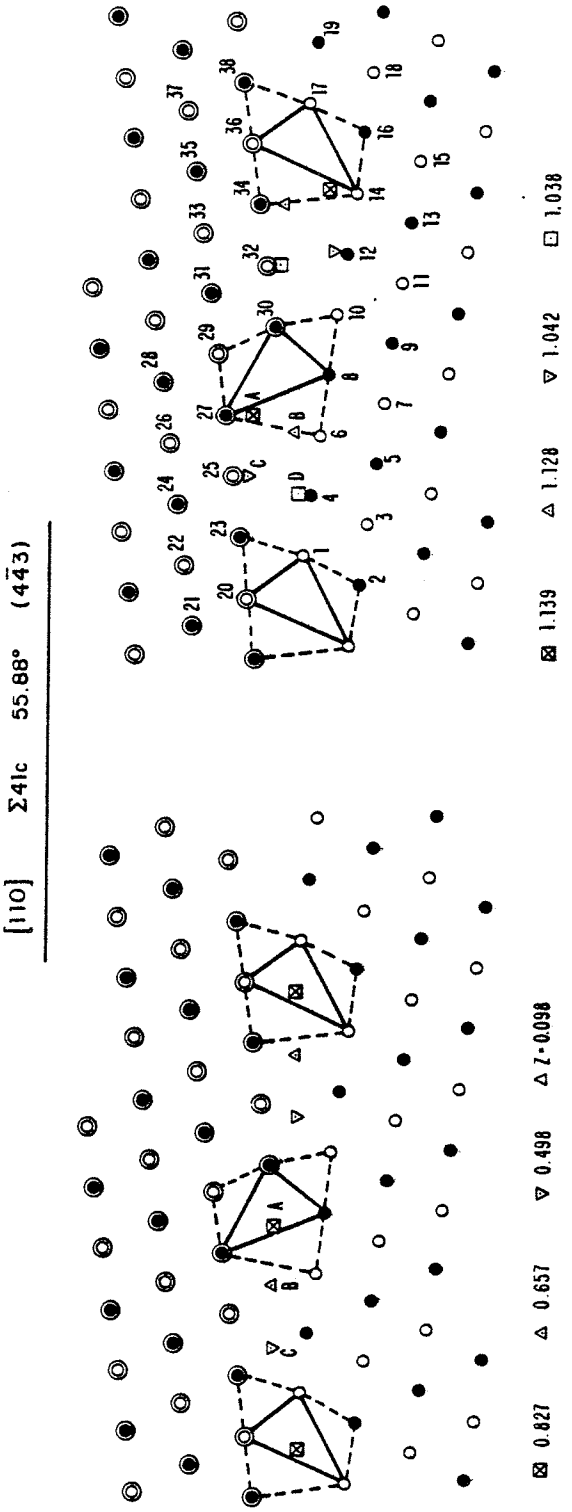
[110] Σ11 50.48° $(3\bar{3}2)$ $\Delta Z = 0.13690$

$$V^{EX} = 0.34118$$

Contacts: 7-21, 7-23, 11-29, 13-29

Interstitials	x	y	z	d	Touching
A	0.62534	2.12131	0.12534	0.76719	3,5,7,21
B	0.24551	1.33741	0.63690	0.54128	1,3,19,19'

Substitutionals		x	y	z	d	Touching
A	3	0.77411	1.57394	0.5	1.07513	1,1',3',3",5,5',19
B	19	0.06667	1.66822	0.13690	1.06637	3,17,17',19',19",21,21'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	-0.70711	0.50000
3	1.00000	0.00000	0.00000
4	0.50000	0.70711	0.50000
5	1.50000	0.70711	0.50000
6	1.00000	1.41421	0.00000
7	2.00000	1.41421	0.00000
8	1.50000	2.12132	0.50000
9	2.50000	2.12132	0.50000
10	2.00000	2.82843	0.00000
11	3.00000	2.82843	0.00000
12	2.50000	3.53553	0.50000
13	3.50000	3.53553	0.50000
14	3.00000	4.24264	0.00000
15	4.00000	4.24264	0.00000
16	3.50000	4.94975	0.50000
17	3.00000	5.65685	0.00000
18	4.00000	5.65685	0.00000
19	3.50000	6.36396	0.50000
20	-0.97710	-0.18892	0.09794
21	-1.84295	-0.17168	0.59794
22	-1.53807	0.63891	0.09794
23	-0.67222	0.62166	0.59794
24	-1.23319	1.44949	0.59794
25	-0.36734	1.43225	0.09794
26	-0.92832	2.26008	0.09794
27	-0.06246	2.24283	0.59794
28	-0.62344	3.07067	0.59794
29	0.24242	3.05342	0.09794
30	1.10827	3.03617	0.59794
31	0.54729	3.86401	0.59794
32	1.41315	3.84676	0.09794
33	0.85217	4.67459	0.09794
34	1.71803	4.65735	0.59794
35	1.15705	5.48518	0.59794
36	2.02290	5.46793	0.09794
37	1.46193	6.29576	0.09794
38	2.32778	6.27852	0.59794

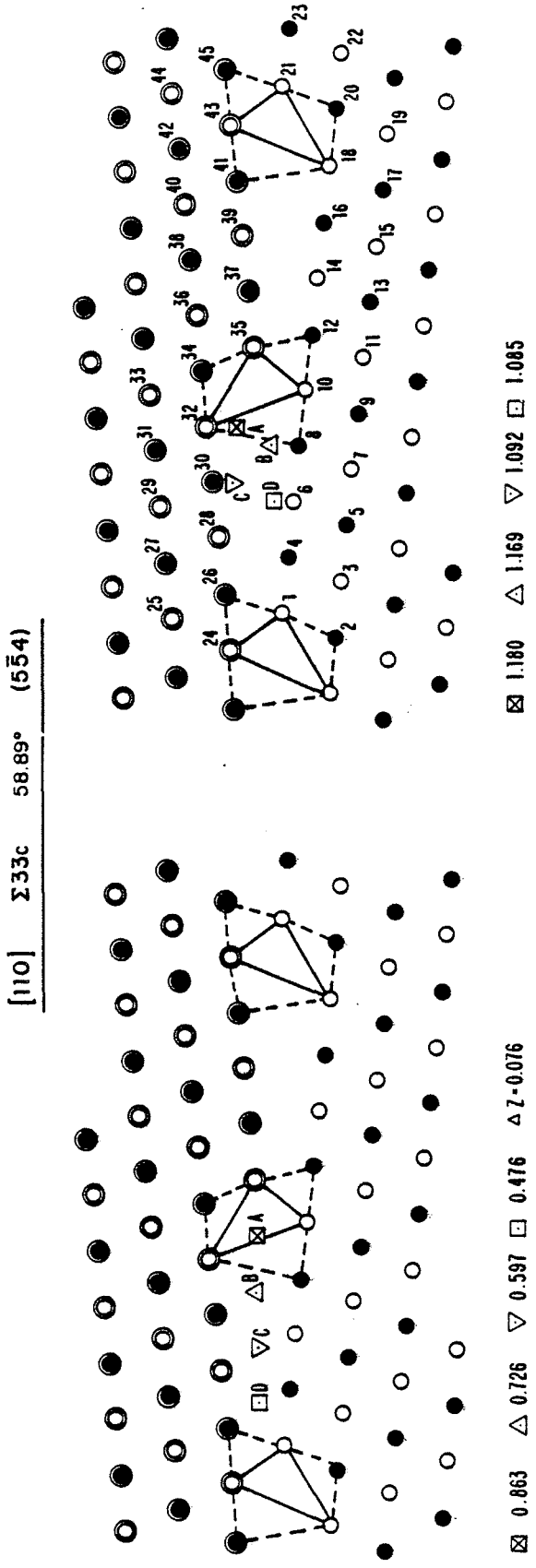
[110] $\Sigma 41c$ 55.88° $(44\bar{3})$ $\Delta z = 0.09794$

$V^{EX} = 0.37375$

Contacts: 1-20, 1-23, 8-30, 10-30

Interstitials	x	y	z	d	Touching
A	0.75232	2.30096	0.00690	0.82700	8,27,29,30
B	0.35006	1.53125	0.5	0.65664	4,6,6',25,27
C	-0.05528	0.75844	0.0	0.49799	4,4',23,25
D	0.30981	1.19514	0.0	0.44824	4,4',6,25

Substitutionals		x	y	z	d	Touching
A	27	0.29307	2.10911	0.59794	1.13943	6,25,25',27',27",29,29'
B	6	0.70363	1.62379	0.0	1.12768	4,4',6',6",8,8',27
C	25	-0.17445	1.35970	0.09794	1.04196	4,23,23',25',25",27,27'
D	4	0.34068	0.81977	0.5	1.03772	1,1',4',4",6,6',25



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	-0.70711	0.50000
3	1.00000	0.00000	0.00000
4	0.50000	0.70711	0.50000
5	1.50000	0.70711	0.50000
6	1.00000	1.41421	0.00000
7	2.00000	1.41421	0.00000
8	1.50000	2.12132	0.50000
9	2.50000	2.12132	0.50000
10	2.00000	2.82843	0.00000
11	3.00000	2.82843	0.00000
12	2.50000	3.53553	0.50000
13	3.50000	3.53553	0.50000
14	3.00000	4.24264	0.00000
15	4.00000	4.24264	0.00000
16	3.50000	4.94975	0.50000
17	4.50000	4.94975	0.50000
18	4.00000	5.65685	0.00000
19	5.00000	5.65685	0.00000
20	4.50000	6.36396	0.50000
21	4.00000	7.07107	0.00000
22	5.00000	7.07107	0.00000
23	4.50000	7.77817	0.50000
24	-0.98585	-0.14942	0.07596
25	-1.50100	0.70767	0.07596
26	-0.63737	0.64339	0.57596
27	-1.15252	1.50049	0.57596
28	-0.28888	1.43621	0.07596
29	-0.80403	2.29331	0.07596
30	0.05960	2.22903	0.57596
31	-0.45555	3.08613	0.57596
32	0.40809	3.02184	0.07596
33	-0.10706	3.87894	0.07596
34	0.75657	3.81466	0.57596
35	1.62021	3.75038	0.07596
36	1.10506	4.60748	0.07596
37	1.96869	4.54320	0.57596
38	1.45354	5.40029	0.57596
39	2.31718	5.33601	0.07596
40	1.80203	6.19311	0.07596
41	2.66566	6.12883	0.57596
42	2.15051	6.98593	0.57596
43	3.01415	6.92165	0.07596
44	2.49900	7.77875	0.07596
45	3.36263	7.71446	0.57596

[110] $\Sigma 33c$ 58.89° $(5\bar{5}4)$ $\Delta Z = 0.07596$

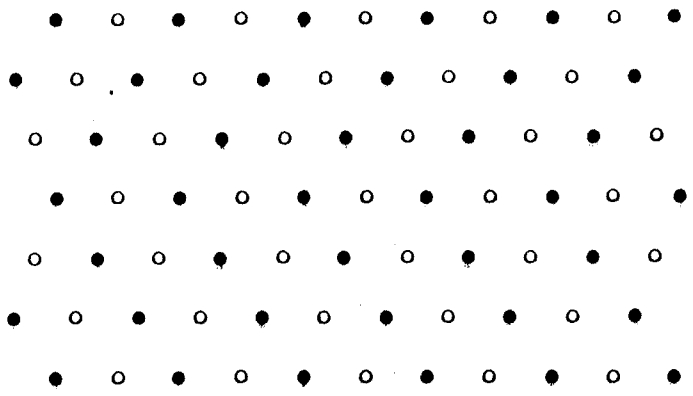
$V^{EX} = 0.39209$

Contacts: 1-24, 1-26', 10-35, 12-35.

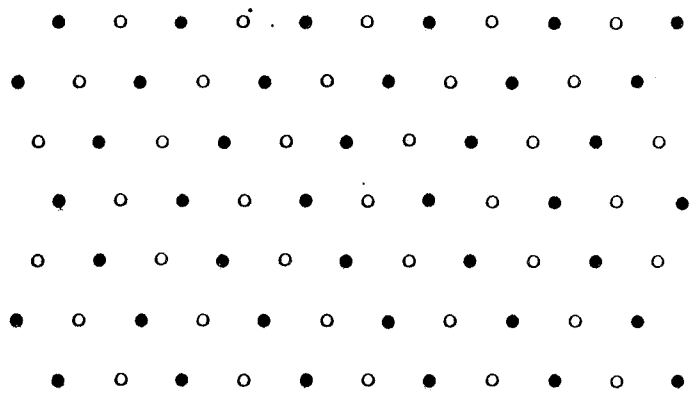
Interstitials	x	y	z	d	Touching
A	0.23490	3.01884	0.50447	0.86251	10,32,34,35
B	0.81067	2.26211	0.0	0.72629	8,8',30,31
C	0.38413	1.50363	0.5	0.59662	6,6',28,30
D	-0.04172	0.74480	0.0	0.47635	4,4',26,28

Substitutionals		x	y	z	d	Touching
A	32	0.80573	2.84706	0.07596	1.18039	8,30,30',32',32",34,34'
B	8	1.15782	2.36327	0.5	1.16852	6,6',8',8",10,10',32
C	30	0.33995	2.10580	0.57596	1.09167	6,28,28',30',30",32,32'
D	6	0.75995	1.58395	0.0	1.08464	4,4',6',6",8,8',30
E	28	-0.13846	1.37009	0.07596	1.02682	4,26,26',28',28",30,30'
F	4	0.37208	0.79756	0.5	1.02440	1,1',4',4",6,6',28

[110] Σ3 70.53° (1$\bar{1}$1)



none > 0.415



none > 1.0

[110] $\Sigma 3$ 70.53° $(1\bar{1}1)$ $\Delta Z = 0.$

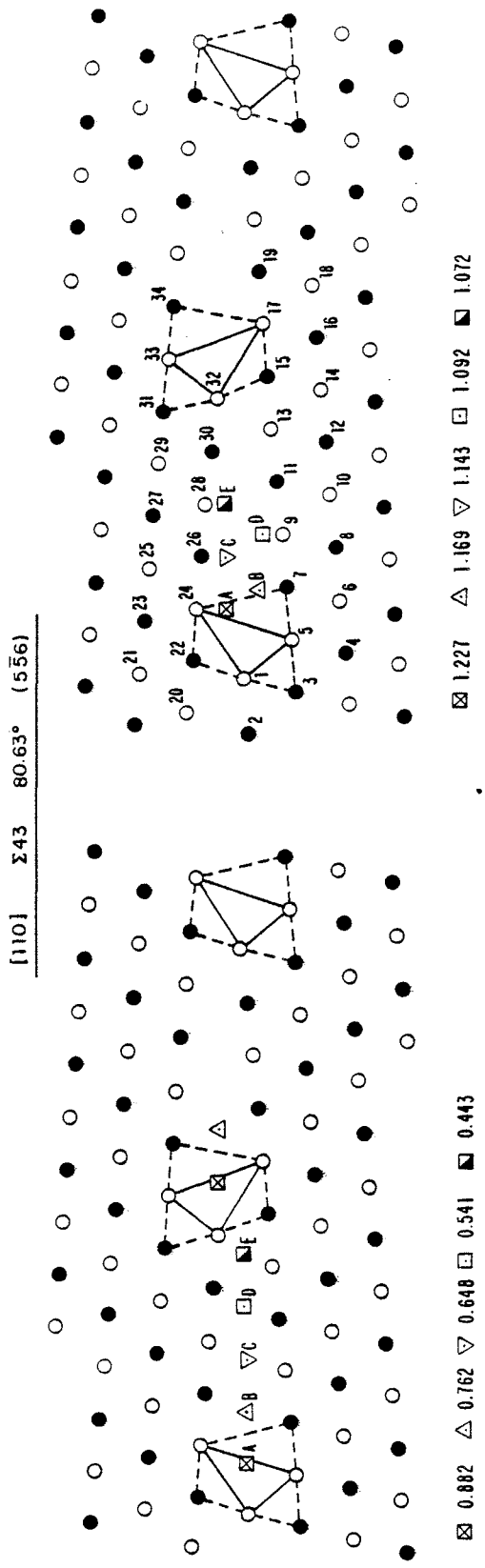
$$V^{EX} = 0.$$

Coherent twin

Interstitials none > 0.415

Substitutionals none > 1.0

Lattices exactly on the coincidence lattice



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.70711	0.50000
3	0.50000	-0.70711	0.50000
4	1.50000	-0.70711	0.50000
5	1.00000	-0.00000	0.00000
6	2.00000	-0.00000	0.00000
7	1.50000	0.70711	0.50000
8	2.50000	0.70711	0.50000
9	2.00000	1.41421	0.00000
10	3.00000	1.41421	0.00000
11	2.50000	2.12132	0.50000
12	3.50000	2.12132	0.50000
13	3.00000	2.82843	0.00000
14	4.00000	2.82843	0.00000
15	3.50000	3.53553	0.50000
16	4.50000	3.53553	0.50000
17	4.00000	4.24264	0.00000
18	5.00000	4.24264	0.00000
19	4.50000	4.94975	0.50000
20	-1.01951	0.15798	0.00000
21	-1.18230	1.14464	0.00000
22	-0.40323	0.76642	0.50000
23	-0.56602	1.75308	0.50000
24	0.21305	1.37486	0.00000
25	0.05026	2.36152	0.00000
26	0.82933	1.98330	0.50000
27	0.66654	2.96996	0.50000
28	1.44560	2.59174	0.00000
29	1.28281	3.57840	0.00000
30	2.06188	3.20019	0.50000
31	1.89909	4.18685	0.50000
32	2.67816	3.80863	0.00000
33	2.51537	4.79529	0.00000
34	3.13165	5.40373	0.50000

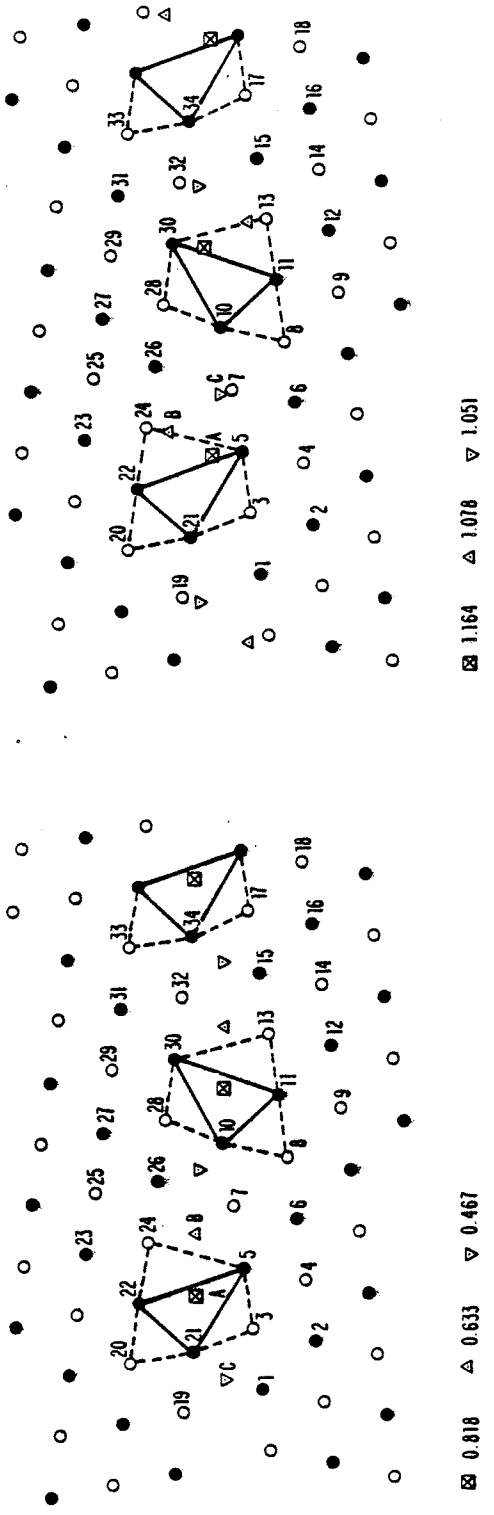
[110] $\Sigma 43$ 80.63° $(5\bar{5}6)$ $\Delta z = 0.0$

$V^{EX} = 0.38819$

Contacts: 1-22, 1-22', 15-32, 15'-32.

Interstitials	x	y	z	d	Touching
A	0.52957	0.64338	0.5	0.88175	5,5',22,24,24'
B	1.09157	1.30679	0.0	0.76231	7,7',24,26,26'
C	1.65346	1.97033	0.5	0.64846	9,9',26,28,28'
D	2.21516	2.63404	0.0	0.54145	11,11',28,30,30'
E	-0.51982	0.01401	0.5	0.44279	1,1',2,20,20'
F	1.98967	2.12862	0.0	0.42897	9,11,11',28

Substitutionals		x	y	z	d	Touching
A	24	0.55740	1.02607	0.0	1.22731	7,7',22,22',24',24",26,26'
B	7	1.15721	0.94950	0.5	1.16911	5,5',7',7",9,9',26
C	26	1.09959	1.70956	0.5	1.14287	9,9',24,24',26',26",28,28'
D	9	1.74985	1.59110	0.0	1.09175	7,7',9',9",11,11',28
E	28	1.63603	2.39886	0.0	1.07216	11,11',26,26',28',28",30,30'
F	11	2.35182	2.22609	0.5	1.03267	9,9',11',11",13,13",30
G	30	2.16391	3.09684	0.5	1.02098	13,13',28,28',30',30",32,32'
H	13	2.96828	2.85085	0.0	1.00151	11,11',13',13",15,15',32



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.0	0.0	0.0
3	0.5	0.70711	0.5
4	1.5	0.70711	0.5
5	1.0	1.41421	0.0
6	2.0	1.41421	0.0
7	1.5	2.12132	0.5
8	2.5	2.12132	0.5
9	3.5	2.12132	0.5
10	2.0	2.82842	0.0
11	3.0	2.82842	0.0
12	4.0	2.82842	0.0
13	3.5	3.5355	0.5
14	4.5	3.5355	0.5
15	4.0	4.24263	0.0
16	5.0	4.24263	0.0
17	4.5	4.9497	0.5
18	5.5	4.9497	0.5
19	-0.9912	0.4623	0.5
20	-1.0499	1.4606	0.5
21	-0.3146	1.0030	0.0
22	-0.3734	2.0013	0.0
23	-0.4322	2.9996	0.0
24	0.3032	2.5420	0.5
25	0.2444	3.5403	0.5
26	0.9797	3.0827	0.0
27	0.9209	4.0810	0.0
28	1.6563	3.6234	0.5
29	1.5975	4.6217	0.5
30	2.3329	4.1641	0.0
31	2.2740	5.1624	0.0
32	3.0094	4.7048	0.5
33	2.9506	5.7031	0.5
34	3.6860	5.2455	0.0

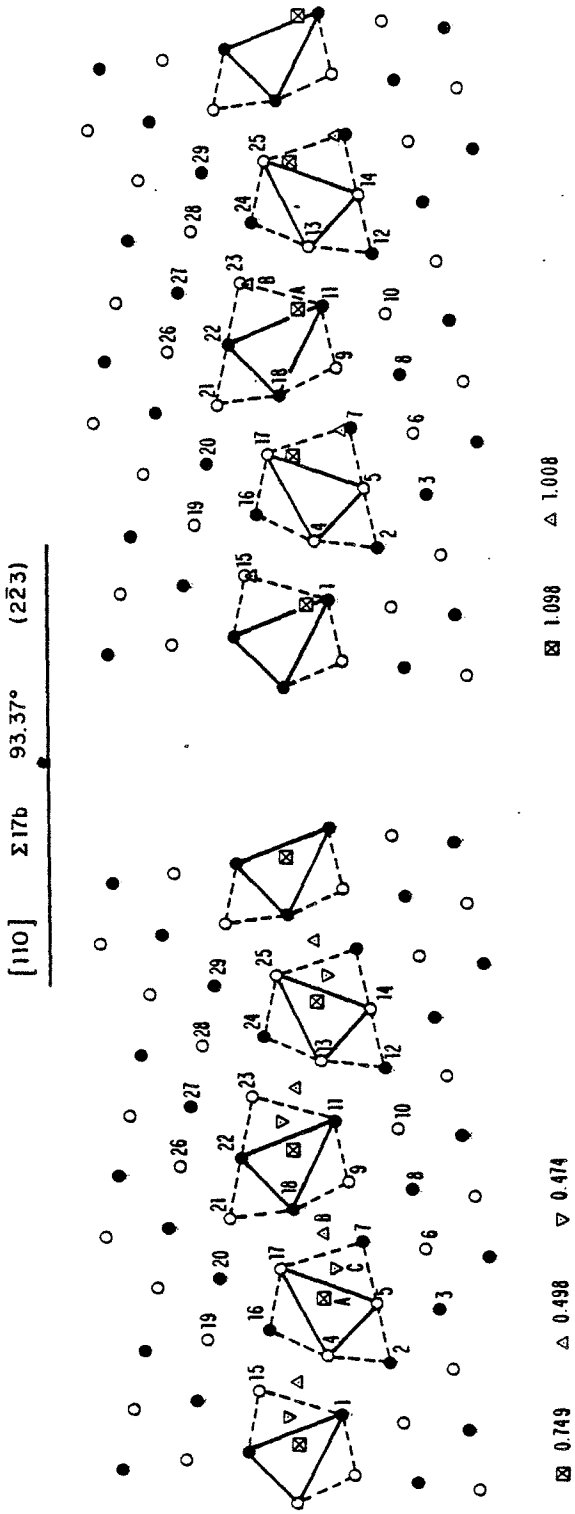
[110] $\Sigma 17b$ 86.63° $(3\bar{3}4)$ $\Delta Z = 0.0$

$V^{EX} = 0.3487$

Contacts: 3-21, 3-21', 10-28, 10-28'

Interstitials	x	y	z	d	Touching
A	0.26035	1.58389	0.5	0.81755	3,5,5',22,22'
B	0.86197	2.21891	0.0	0.63292	5,7,7',24,24'
C	-0.25834	0.47010	0.5	0.46661	1,1',19,21,21'

Substitutionals		x	y	z	d	Touching
A	5	0.66290	1.65258	0.0	1.16374	3,3',5',5",7,7',24,24'
B	24	0.47999	2.32063	0.5	1.07871	7,22,22',24',24",26,26'
C	7	1.31460	2.25240	0.5	1.05091	5,5',7',7",9,9',26,26'
D	26	1.01917	3.03330	0.0	1.00399	10,24,24',26',26",28,28'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.0	0.0	0.
3	2.	0.	0.
4	0.5	0.70711	0.5
5	1.5	0.70711	0.5
6	2.5	0.70711	0.5
7	2.	1.41421	0.
8	3.	1.41421	0.
9	2.5	2.12132	0.5
10	3.5	2.12132	0.5
11	3.	2.82843	0.
12	4.	2.82843	0.
13	3.5	3.53553	0.5
14	4.5	3.53553	0.5
15	-0.50972	1.07096	0.5
16	0.22558	1.52850	0.
17	0.96087	1.98604	0.5
18	1.69617	2.44358	0.
19	-0.45089	2.06923	0.5
20	0.28440	2.52677	0.
21	1.01970	2.98431	0.5
22	1.75499	3.44185	0.
23	2.49029	3.89939	0.5
24	3.22558	4.35692	0.
25	3.96088	4.81446	0.5
26	1.07852	3.98258	0.5
27	1.81382	4.44012	0.
28	2.54911	4.89765	0.5
29	3.28441	5.35519	0.

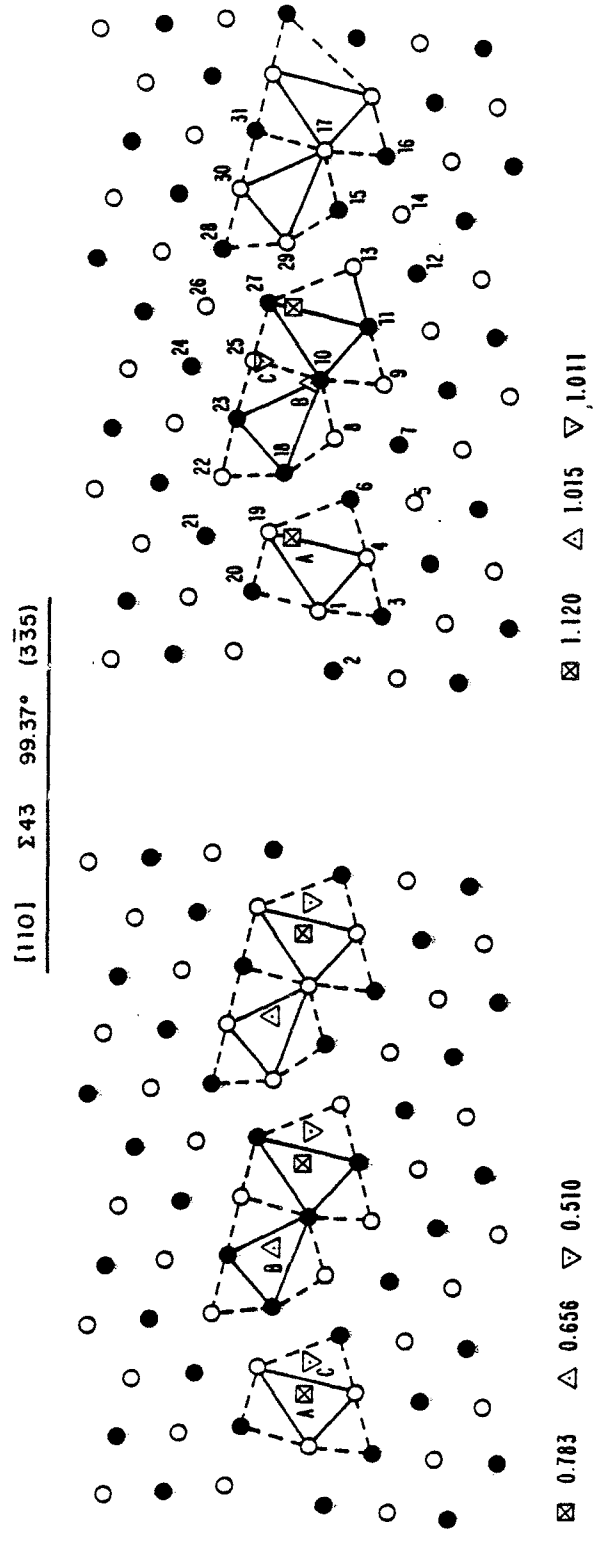
[110] $\Sigma 17b$ 93.37° $(2\bar{2}3)$ $\Delta Z = 0.0$

$$V^{EX} = 0.3042$$

Contacts: 4-16, 4-16', 9-18, 9-18'

Interstitials	x	y	z	d	Touching
A	1.06275	1.27582	0.0	0.74894	5,5',16,17,17'
B	1.70306	1.88609	0.5	0.49778	7,7',17,18,18'
C	1.45933	1.44317	0.5	0.47399	5,7,7',17

Substitutionals		x	y	z	d	Touching
A	11	2.74081	3.01169	0.0	1.09834	9,9',11',11",13,13',23,23'
B	23	2.53794	3.82278	0.5	1.00812	13,22,22',23',23",24,24'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.70711	0.50000
3	0.50000	-0.70711	0.50000
4	1.00000	-0.00000	0.00000
5	2.00000	-0.00000	0.00000
6	1.50000	0.70711	0.50000
7	2.50000	0.70711	0.50000
8	2.00000	1.41421	0.00000
9	3.00000	1.41421	0.00000
10	2.50000	2.12132	0.50000
11	3.50000	2.12132	0.50000
12	4.50000	2.12132	0.50000
13	4.00000	2.82843	0.00000
14	5.00000	2.82843	0.00000
15	4.50000	3.53553	0.50000
16	5.50000	3.53553	0.50000
17	5.00000	4.24264	0.00000
18	1.16667	1.64992	0.50000
19	0.38760	1.27170	0.00000
20	-0.39147	0.89348	0.50000
21	-0.22868	1.88014	0.50000
22	0.55039	2.25836	0.00000
23	1.32946	2.63658	0.50000
24	1.49225	3.62324	0.50000
25	2.10853	3.01480	0.00000
26	2.27132	4.00146	0.00000
27	2.88760	3.39302	0.50000
28	3.05039	4.37968	0.50000
29	3.66667	3.77124	0.00000
30	3.82946	4.75790	0.00000
31	4.60853	5.13612	0.50000

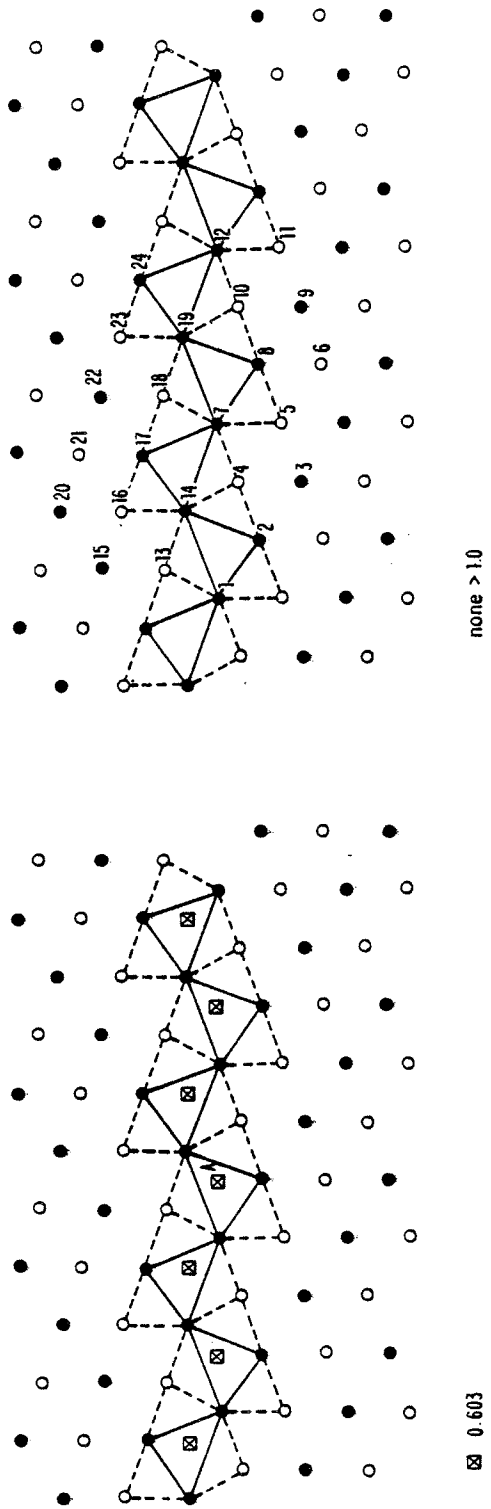
[110] $\Sigma 43$ 99.37° $(3\bar{3}5)$ $\Delta Z = 0$

$v^{EX} = 0.32277$

Contacts: 6-18, 8-18, 8-18'.

Interstitials	x	y	z	d	Touching
A	0.5	0.54252	0.5	0.78250	1,1',4,4',19,19'
B	1.84848	2.22846	0.0	0.65644	8,10,10',23,23'
C	0.93950	0.75243	0.0	0.51032	4,6,6',19

Substitutionals		x	y	z	d	Touching
A	19	0.54111	0.95550	0.0	1.11995	4,18,18',19',19",20,20'
B	10	2.40152	2.19096	0.5	1.01450	8,8',10',10",25,25'
C	25	2.15368	2.92179	0.0	1.01066	10,10',23,23',25',25",27,27'



	X	Y	Z
1	2.00000	1.41421	0.00000
2	3.	1.41421	0.
3	4.	1.41421	0.
4	3.5	2.12132	0.5
5	4.5	2.12132	0.5
6	5.5	2.12132	0.5
7	4.	2.82843	0.
8	5.	2.82843	0.
9	6.	2.82843	0.
10	5.5	3.53553	0.5
11	6.5	3.53553	0.5
12	6.	4.24264	0.
13	1.89238	2.27353	0.5
14	2.72571	2.50923	0.
15	1.39238	2.98064	0.
16	2.22571	3.21634	0.5
17	3.05904	3.45204	0.
18	3.89237	3.68774	0.5
19	4.72570	3.92344	0.
20	1.72571	3.92344	0.
21	2.55904	4.15915	0.5
22	3.39237	4.39485	0.
23	4.22570	4.63055	0.5
24	5.05903	4.86625	0.

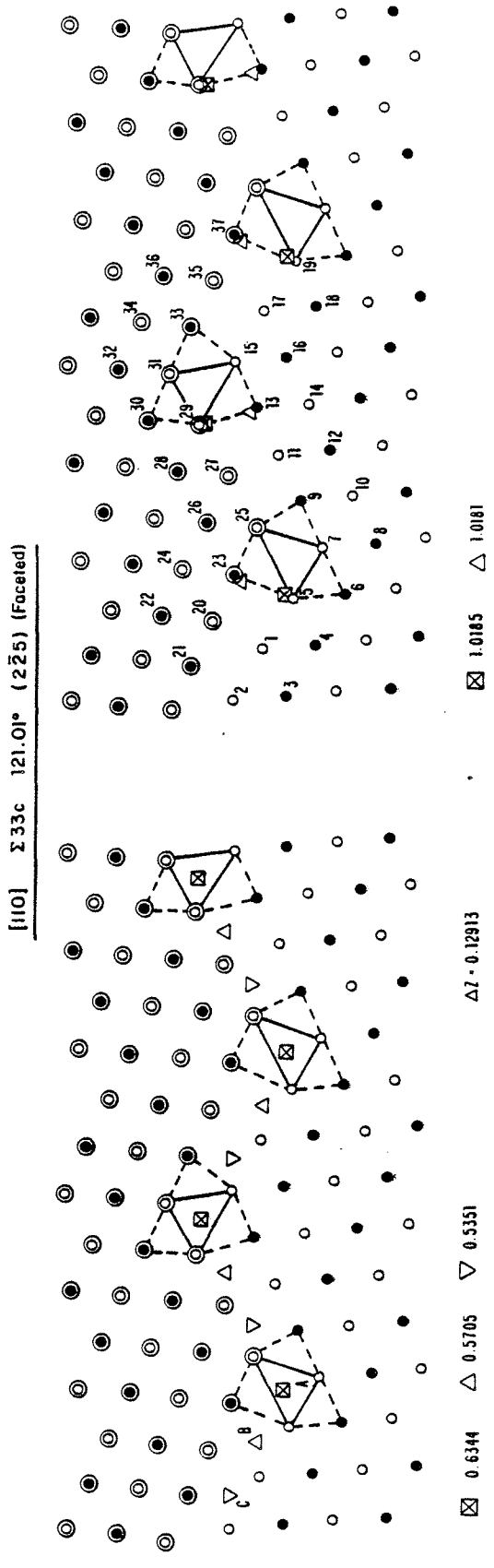
[110] $\Sigma 3$ 109.47° $(1\bar{1}2)$ $\Delta Z = 0.0$

$V^{EX} = 0.2092$

Contacts: 4-14, 4-14', 7-18, 7-18'

Interstitials	x	y	z	d	Touching
A	2.59924	1.89568	0.5	0.60302	8,8',18,19,19'

Substitutionals none > 1.0



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-1.00000	-0.00000	0.00000
3	-0.50000	-0.70711	0.50000
4	0.50000	-0.70711	0.50000
5	1.00000	-0.00000	0.00000
6	1.50000	-0.70711	0.50000
7	2.00000	0.00000	0.00000
8	2.50000	-0.70711	0.50000
9	2.50000	0.70711	0.50000
10	3.00000	0.00000	0.00000
11	3.00000	1.41421	0.00000
12	3.50000	0.70711	0.50000
13	3.50000	2.12132	0.50000
14	4.00000	1.41421	0.00000
15	4.00000	2.82843	0.00000
16	4.50000	2.12132	0.50000
17	5.00000	2.82843	0.00000
18	5.50000	2.12132	0.50000
19	6.00000	2.82843	0.00000
20	-0.05993	0.98981	0.12913
21	-0.92356	0.92553	0.62913
22	-0.40841	1.78263	0.62913
23	0.80371	1.05410	0.62913
24	0.45523	1.84691	0.12913
25	1.66735	1.11838	0.12913
26	1.31886	1.91120	0.62913
27	2.18250	1.97548	0.12913
28	1.83401	2.76830	0.62913
29	2.69765	2.83258	0.12913
30	2.34917	3.62540	0.62913
31	3.21280	3.68968	0.12913
32	2.86432	4.48250	0.62913
33	4.07644	3.75396	0.62913
34	3.72795	4.54678	0.12913
35	4.94008	3.81824	0.12913
36	4.59159	4.61106	0.62913
37	5.80371	3.88253	0.62913

[110] Σ33c 121.01° $(2\bar{2}5)$ $\Delta z = 0.12913$

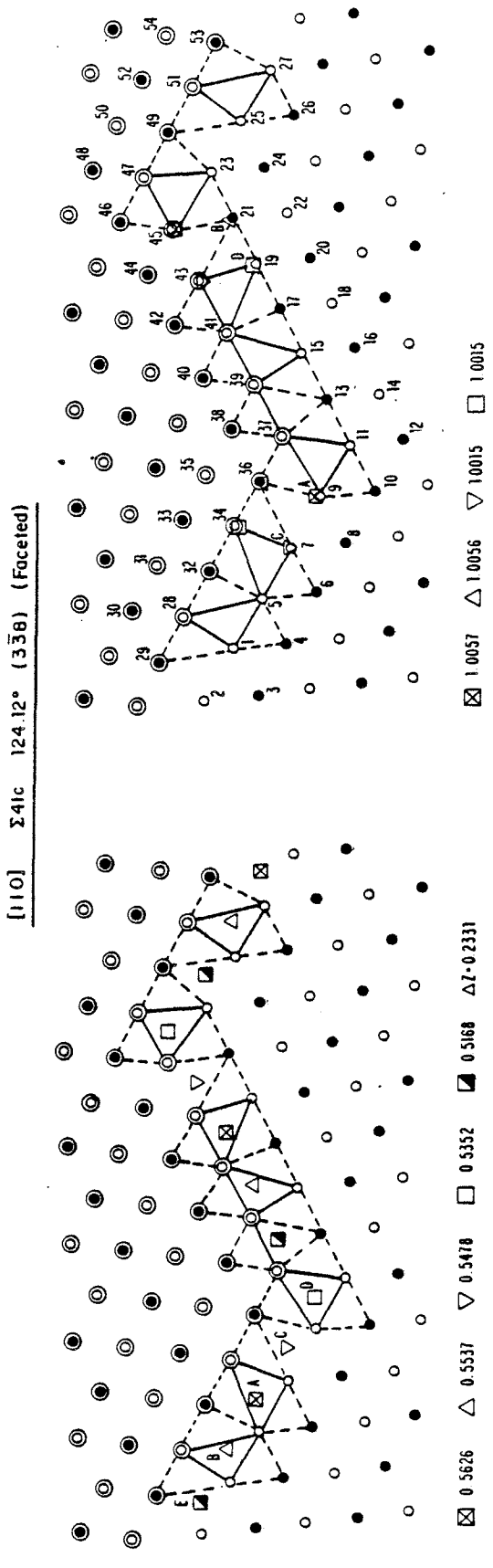
Faceted

$V^{EX} = 0.30932$

Contacts: 1-20, 11-27, 2-21, 9-25

Interstitials	x	y	z	d	Touching
A	1.5	0.40967	0.5	0.63441	5,5',7,7',25
B	0.5	0.34154	0.5	0.57054	1,1',5,5',23
C	-0.5	0.29858	0.5	0.53512	1,1',2,2',21

Substitutionals		x	y	z	d	Touching
A	5	1.0	0.13623	0.0	1.01847	1,5,5',7,23
B	13	3.38998	2.19911	0.5	1.01807	11,11',13',13'',15,15',29



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-1.00000	-0.00000	0.00000
3	-0.50000	-0.70711	0.50000
4	0.50000	-0.70711	0.50000
5	1.00000	-0.00000	0.00000
6	1.50000	-0.70711	0.50000
7	2.00000	0.00000	0.00000
8	2.50000	-0.70711	0.50000
9	3.00000	0.00000	0.00000
10	3.50000	-0.70711	0.50000
11	4.00000	0.00000	0.00000
12	4.50000	-0.70711	0.50000
13	4.50000	0.70711	0.50000
14	5.00000	0.00000	0.00000
15	5.00000	1.41421	0.00000
16	5.50000	0.70711	0.50000
17	5.50000	2.12132	0.50000
18	6.00000	1.41421	0.00000
19	6.00000	2.82843	0.00000
20	6.50000	2.12132	0.50000
21	6.50000	3.53554	0.50000
22	7.00000	2.82843	0.00000
23	7.00000	4.24264	0.00000
24	7.50000	3.53554	0.50000
25	8.00000	4.24264	0.00000
26	8.50000	3.53554	0.50000
27	9.00000	4.24264	0.00000
28	0.11773	0.95651	0.26689
29	-0.74812	0.93926	0.76689
30	-0.18714	1.76709	0.76689
31	0.67871	1.78434	0.26689
32	0.98359	0.97376	0.76689
33	1.54456	1.80159	0.76689
34	1.84944	0.99100	0.26689
35	2.41042	1.81883	0.26689
36	2.71529	1.00825	0.76689
37	3.58115	1.02549	0.26689
38	3.27627	1.83608	0.76689
39	4.14212	1.85333	0.26689
40	3.83725	2.66391	0.76689
41	4.70310	2.68116	0.26689
42	4.39822	3.49174	0.76689
43	5.26408	3.50899	0.26689
44	4.95920	4.31958	0.76689
45	5.82505	4.33682	0.26689
46	5.52017	5.14741	0.76689
47	6.38603	5.16466	0.26689
48	6.08115	5.97524	0.76689
49	7.25188	5.18190	0.76689
50	6.94700	5.99249	0.26689
51	8.11774	5.19915	0.26689
52	7.81286	6.00973	0.76689
53	8.98359	5.21639	0.76689
54	8.67871	6.02698	0.26689

[110] $\Sigma 41c$ 124.12° $(3\bar{3}8)$ $\Delta z = 0.23311$

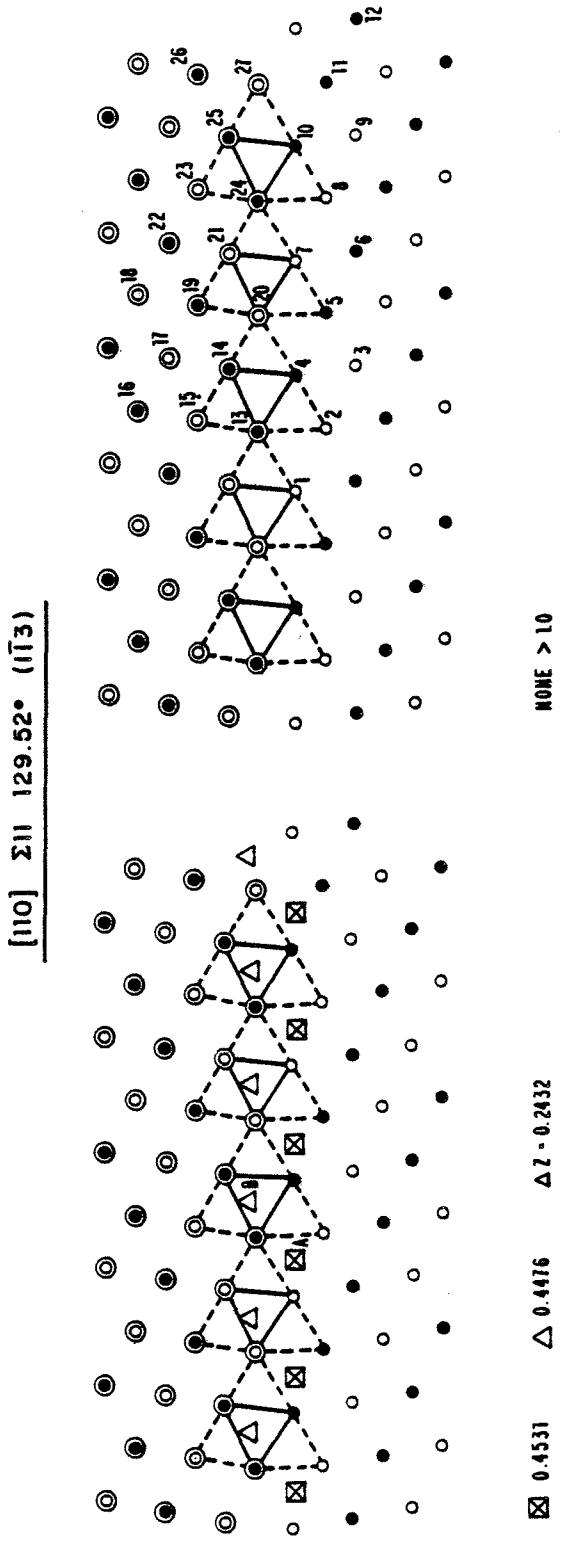
Faceted

$V^{EX} = 0.27305$

Contacts: 1-28, 15-39, 2-29, 13-37

Interstitials	x	y	z	d	Touching
A	1.5	0.33226	0.5	0.56255	5,5',7,7',34
B	0.5	0.32168	0.5	0.55371	1,1',5,5',28
C	2.5	0.31448	0.5	0.54777	7,7',9,9',36
D	3.5	0.29867	0.5	0.53519	9,9',11,1',37
E	-0.5	0.27415	0.5	0.51679	1,1',2,2',29

Substitutionals		x	y	z	d	Touching
A	9	3.0	0.07536	0.0	1.00567	7,9',9'',11,36
B	21	6.43880	3.57881	0.5	1.00561	19,19',21',21'',23,23',45
C	7	2.0	0.03833	0.0	1.00147	5,7',7'',9,34
D	19	5.96879	2.85050	0.0	1.00146	17,17',19',19'',21,21',43



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	2.00000	0.00000	0.00000
4	1.50000	0.70711	0.50000
5	2.50000	0.70711	0.50000
6	3.50000	0.70711	0.50000
7	3.00000	1.41421	0.00000
8	4.00000	1.41421	0.00000
9	5.00000	1.41421	0.00000
10	4.50000	2.12132	0.50000
11	5.50000	2.12132	0.50000
12	6.50000	2.12132	0.50000
13	0.54066	0.85034	0.74322
14	1.17703	1.62173	0.74322
15	0.31339	1.68601	0.24322
16	0.08612	2.52168	0.74322
17	0.94975	2.45740	0.24322
18	1.58612	3.22879	0.24322
19	1.81339	2.39312	0.74322
20	2.04066	1.55744	0.24322
21	2.67703	2.32883	0.24322
22	2.44975	3.16451	0.74322
23	3.31339	3.10022	0.24322
24	3.54066	2.26455	0.74322
25	4.17703	3.03594	0.74322
26	4.81339	3.80733	0.74322
27	5.04066	2.97166	0.24322

[110] $\Sigma 11$ 129.52° $(1\bar{1}3)$ $\Delta z = 0.24322$

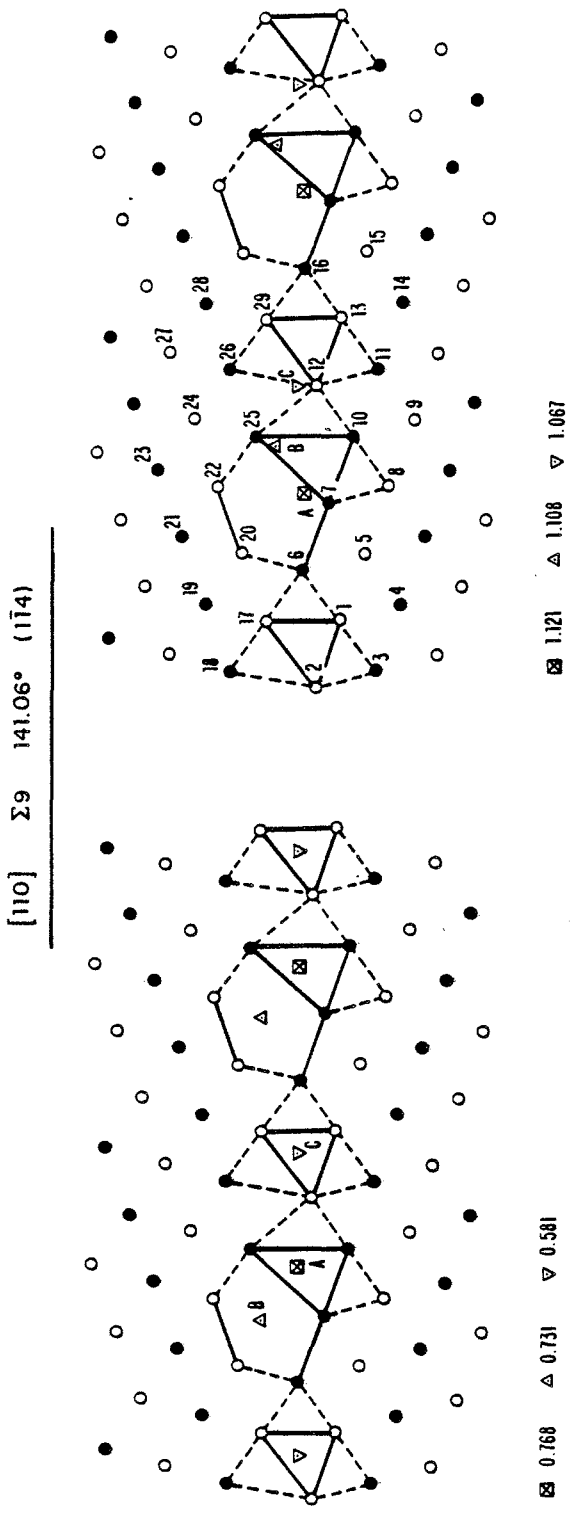
$V^{EX} = 0.12596$

Contacts: 4-14, 7-20, 5-20

Interstitials	x	y	z	d	Touching
A	0.5	0.16692	0.5	0.45308	1,1',2,2',13
B	0.97800	1.13774	0.24322	0.44757	4,13,13',14,14'

Substitutionals

None >1.0.



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-1.00000	-0.00000	0.00000
3	-0.50000	-0.70711	0.50000
4	0.50000	-0.70711	0.50000
5	1.00000	-0.00000	0.00000
6	0.50000	0.70711	0.50000
7	1.50000	0.70711	0.50000
8	2.00000	0.00000	0.00000
9	3.00000	0.00000	0.00000
10	2.50000	0.70711	0.50000
11	3.50000	0.70711	0.50000
12	3.00000	1.41421	0.00000
13	4.00000	1.41421	0.00000
14	4.50000	0.70711	0.50000
15	5.00000	1.41421	0.00000
16	4.50000	2.12132	0.50000
17	-0.33333	0.94281	0.00000
18	-1.16667	1.17851	0.50000
19	-0.38889	1.80705	0.50000
20	0.44444	1.57135	0.00000
21	0.38889	2.43559	0.50000
22	1.22222	2.19989	0.00000
23	1.16667	3.06413	0.50000
24	2.00000	2.82843	0.00000
25	2.05556	1.96419	0.50000
26	2.83333	2.59273	0.50000
27	2.77778	3.45697	0.00000
28	3.61111	3.22127	0.50000
29	3.66667	2.35702	0.00000

[110] $\Sigma 9$ 141.06° $(1\bar{1}4)$ $\Delta z = 0.0$

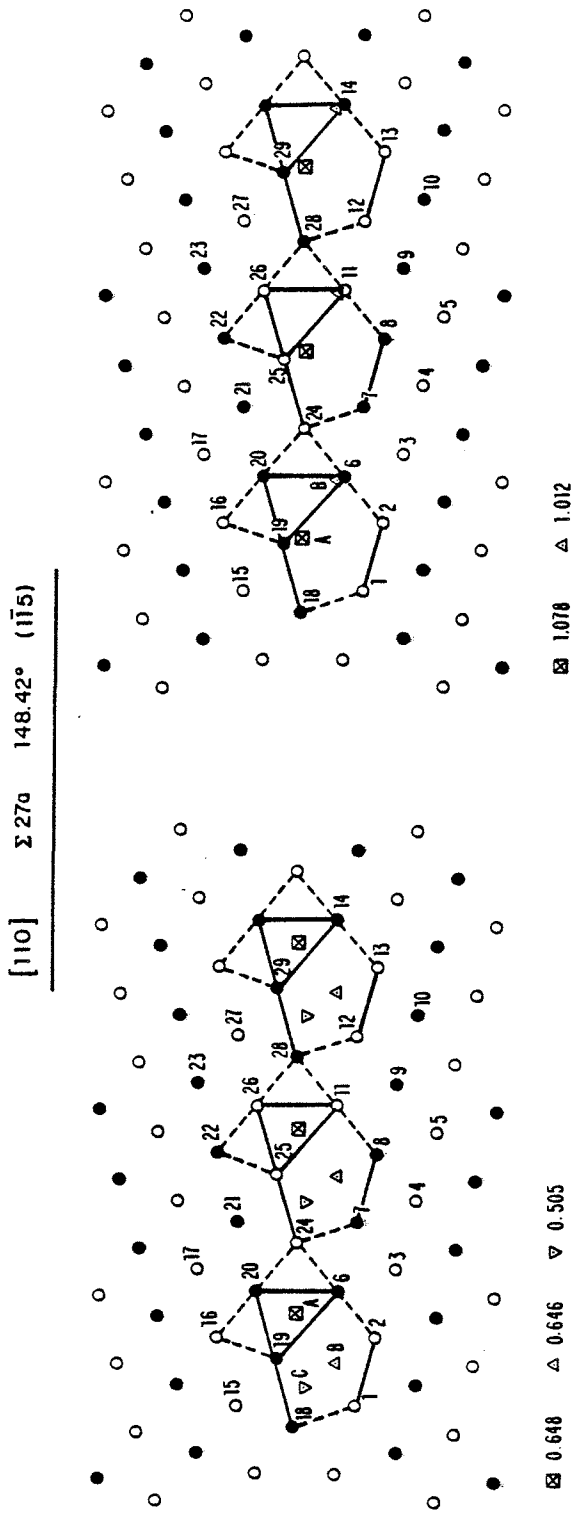
$v^{EX} = 0.37415$

Contacts: 1-17, 6-17, 6'-17

Interstitials	x	y	z	d	Touching
A	2.0	1.23744	0.0	0.76777	7,7',10,10',25,25'
B	1.14705	1.49740	0.5	0.73105	7,20,20',22,22'
C	-0.5	0.35356	0.5	0.58114	1,1',2,2',17,17'
D	1.0	1.02852	0.0	0.55345	6,6',7,7',20
E	2.61539	2.06693	0.0	0.51521	12,25,25',26,26'
F	2.76924	1.87656	0.5	0.43807	12,12',25,26

Substitutionals		x	y	z	d	Touching
A	7	1.5	1.06066	0.5	1.12132	6,7',7",10,25
B	25	2.00002	1.63520	0.5	1.10838	7,10,25',25"
C	12	2.90625	1.65728	0.0	1.06676	12',12",25,25',29

Lattices exactly on the coindicence lattice; CSL sites: 6,16



	X	Y	Z
1	1.00000	0.00000	0.00000
2	2.	0.	0.
3	3.	0.	0.
4	4.	0.	0.
5	5.	0.	0.
6	2.5	0.70711	0.5
7	3.5	0.70711	0.5
8	4.5	0.70711	0.5
9	5.5	0.70711	0.5
10	6.5	0.70711	0.5
11	5.	1.41421	0.
12	6.	1.41421	0.
13	7.	1.41421	0.
14	7.5	2.12132	0.5
15	0.55565	1.57135	0.
16	1.40756	2.09504	0.
17	2.25947	2.61873	0.
18	0.5	0.70711	0.5
19	1.35191	1.23080	0.5
20	2.20382	1.75449	0.5
21	3.05573	2.27818	0.5
22	3.90764	2.80187	0.5
23	4.75955	3.32556	0.5
24	3.0	1.41421	0.
25	3.85181	1.93790	0.
26	4.70382	2.46159	0.
27	5.55573	2.98528	0.
28	5.5	2.12132	0.5
29	6.35181	2.64501	0.5

[110] Σ27a 148.42° $(1\bar{1}5)$ ΔZ = 0.0

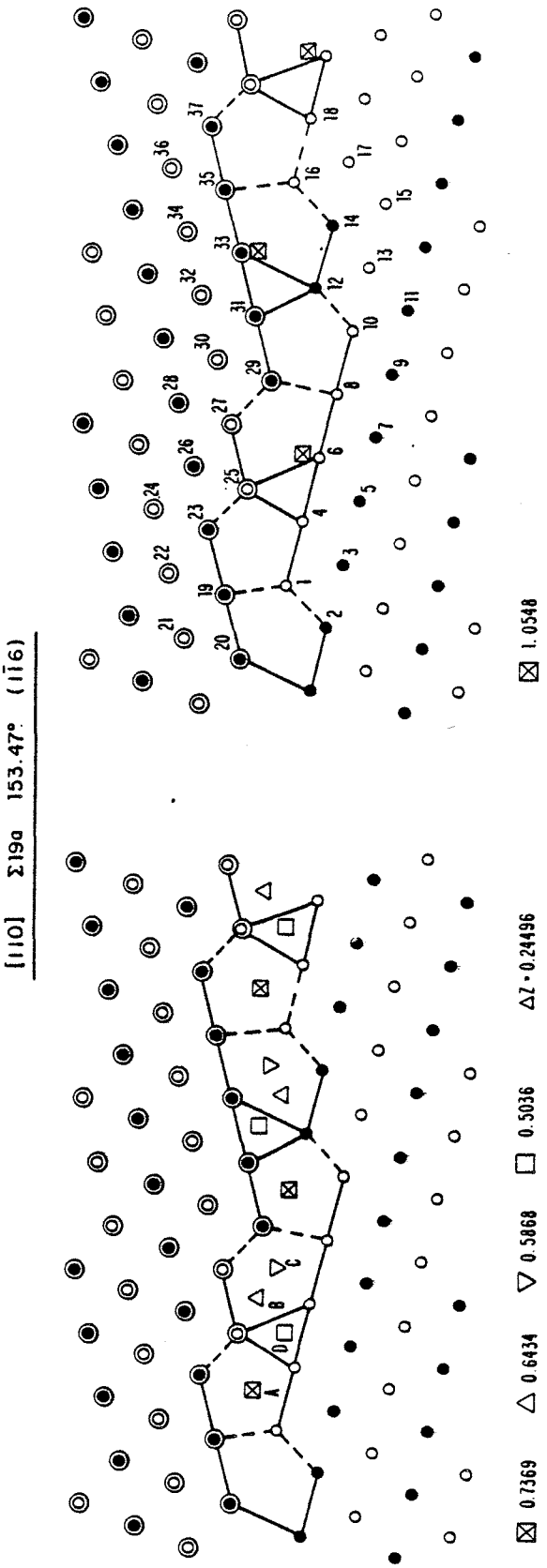
$$v^{EX} = 0.3053$$

Contacts: 6-24, 6-24', 7-24, 7-24'

Interstitials	x	y	z	d	Touching
A	2.00013	1.130846	0.0	0.64844	6,6',19,19',20,20'
B	1.5	0.42119	0.5	0.64609	1,1',2,2',19
C	1.06059	0.749947	0.0	0.50478	1,18,18',19,19'

Substitutionals		x	y	z	d	Touching
A	19	0.98989	1.5	0.5	1.07843	6,18,19',19",20
B	6	0.77010	2.41092	0.5	1.01187	2,2',6',6",19,24,24'

Lattices exactly on the coincidence lattice; CSL sites: 24,28



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.70711	0.50000
3	0.50000	-0.70711	0.50000
4	1.00000	-0.00000	0.00000
5	1.50000	-0.70711	0.50000
6	2.00000	0.00000	0.00000
7	2.50000	-0.70711	0.50000
8	3.00000	0.00000	0.00000
9	3.50000	-0.70711	0.50000
10	4.00000	0.00000	0.00000
11	4.50000	-0.70711	0.50000
12	4.50000	0.70711	0.50000
13	5.00000	0.00000	0.00000
14	5.50000	0.70711	0.50000
15	6.00000	0.00000	0.00000
16	6.00000	1.41421	0.00000
17	6.50000	0.70711	0.50000
18	7.00000	1.41421	0.00000
19	-0.37654	0.89060	0.25504
20	-1.27128	0.44401	0.25504
21	-1.13970	1.29998	0.75504
22	-0.24497	1.74657	0.75504
23	0.51819	1.33720	0.25504
24	0.64977	2.19317	0.75504
25	1.28135	0.92782	0.75504
26	1.41293	1.78379	0.25504
27	2.17609	1.37441	0.75504
28	2.30767	2.23038	0.25504
29	2.93925	0.96503	0.25504
30	3.07082	1.82101	0.75504
31	3.83398	1.41163	0.25504
32	3.96556	2.26760	0.75504
33	4.72872	1.85822	0.25504
34	4.86030	2.71419	0.75504
35	5.62346	2.30482	0.25504
36	5.75504	3.16079	0.75504
37	6.51819	2.75141	0.25504

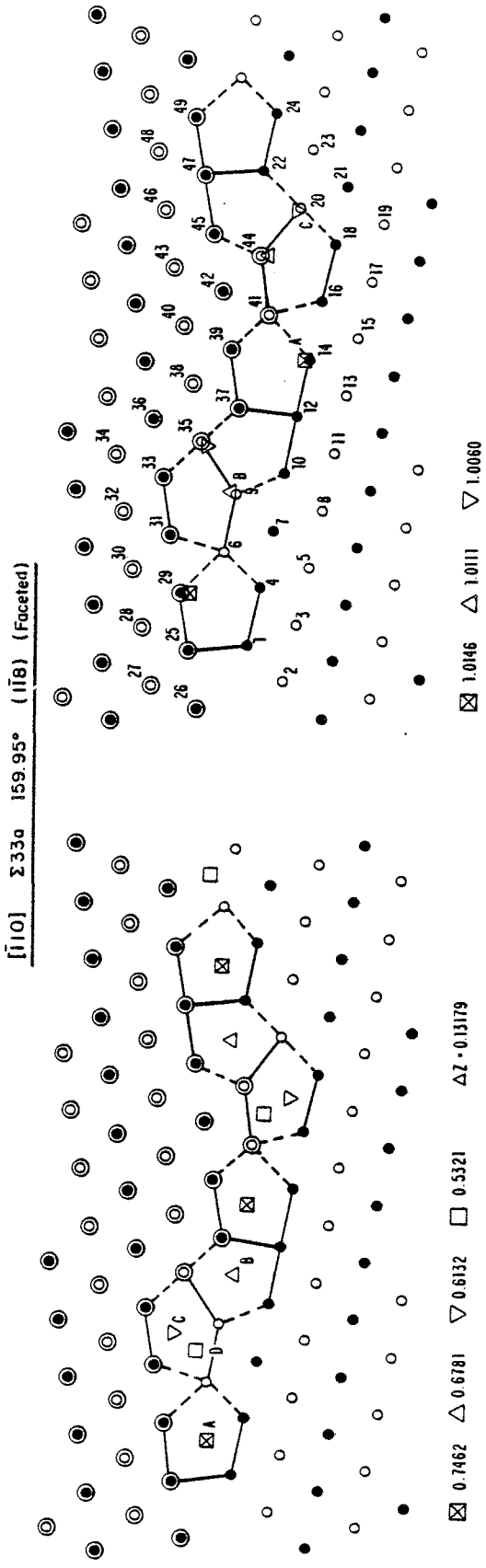
[110] Σ19a 153.47° $(1\bar{1}6)$ $\Delta z = 0.24496$

$V^{EX} = 0.42619$

Contacts: 1-19, 8-29, 4-25, 12-31

Interstitials	x	y	z	d	Touching
A	0.5	0.50427	0.5	0.73680	1,1',4,4',23
B	1.91566	0.77658	0.25504	0.64345	6,25,25',27,27'
C	2.42757	0.62184	0.75504	0.58682	6,27,29,29'
D	1.5	0.25528	0.5	0.50355	4,4',6,6',25

Substitutionals		x	y	z	d	Touching
A	6	2.0	0.23567	0.0	1.05479	4,6',6'',8,25



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.70711	0.50000
3	0.50000	-0.70711	0.50000
4	1.00000	-0.00000	0.00000
5	1.50000	-0.70711	0.50000
6	1.50000	0.70711	0.50000
7	2.00000	0.00000	0.00000
8	2.50000	-0.70711	0.50000
9	2.50000	0.70711	0.50000
10	3.00000	0.00000	0.00000
11	3.50000	-0.70711	0.50000
12	4.00000	0.00000	0.00000
13	4.50000	-0.70711	0.50000
14	5.00000	0.00000	0.00000
15	5.50000	-0.70711	0.50000
16	6.00000	0.00000	0.00000
17	6.50000	-0.70711	0.50000
18	7.00000	0.00000	0.00000
19	7.50000	-0.70711	0.50000
20	7.50000	0.70711	0.50000
21	8.00000	0.00000	0.00000
22	8.00000	1.41421	0.00000
23	8.50000	0.70711	0.50000
24	9.00000	1.41421	0.00000
25	-0.29246	0.94715	0.13179
26	-1.23185	0.60431	0.13179
27	-1.00458	1.43998	0.63179
28	-0.06519	1.78282	0.63179
29	0.64694	1.28999	0.13179
30	0.87421	2.12566	0.63179
31	1.58633	1.63283	0.13179
32	1.81360	2.46850	0.63179
33	2.52572	1.97567	0.13179
34	2.75300	2.81134	0.63179
35	3.23784	1.48284	0.63179
36	3.46512	2.31851	0.13179
37	3.94997	0.99001	0.13179
38	4.17724	1.82568	0.63179
39	4.88936	1.33285	0.13179
40	5.11663	2.16852	0.63179
41	5.60148	0.84002	0.63179
42	5.82875	1.67569	0.13179
43	6.05603	2.51136	0.63179
44	6.54088	1.18286	0.63179
45	6.76815	2.01853	0.13179
46	6.99542	2.85420	0.63179
47	7.70754	2.36137	0.13179
48	7.93482	3.19704	0.63179
49	8.64694	2.70421	0.13179

[110] Σ33a 159.95° $(1\bar{1}8)$ $\Delta z = 0.13179$

Faceted

$v^{EX} = 0.42017$

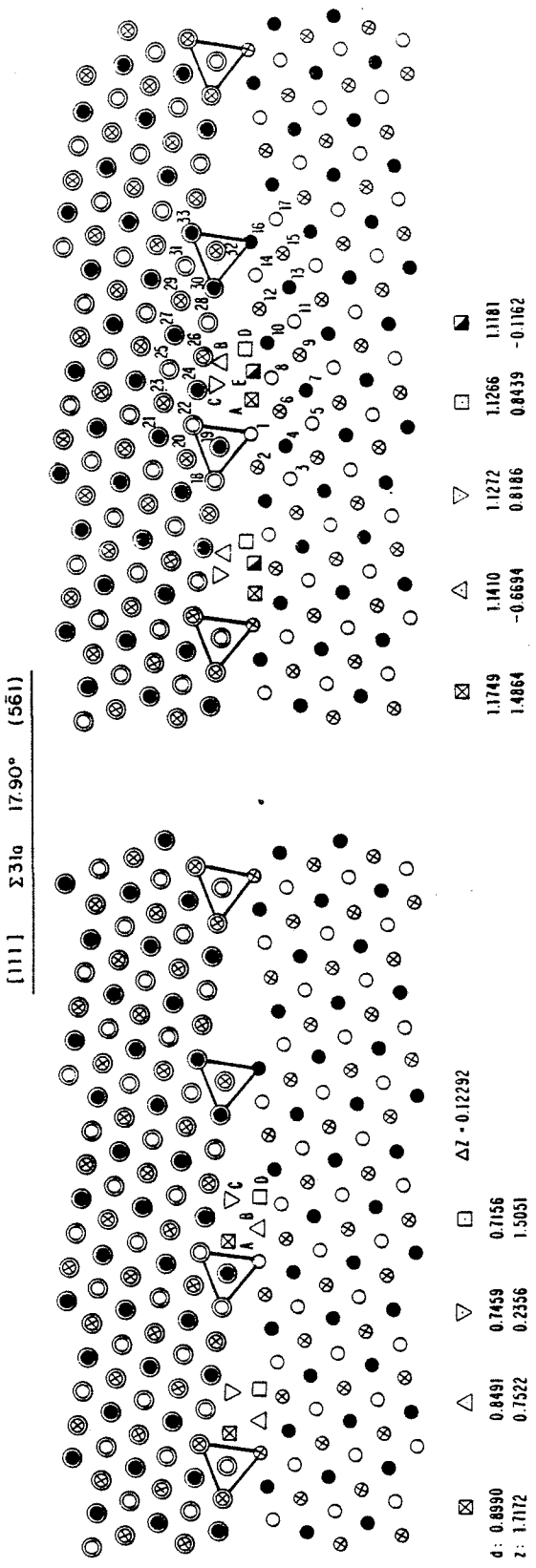
Contacts: 1-25, 6-31, 12-37, 16-41

Interstitials	x	y	z	d	Touching
A	0.5	0.51211	0.5	0.74615	1,1',4,4',29
B	3.33255	0.65037	0.58722	0.67806	9,10,35,37
C	2.18909	1.43965	0.63179	0.61324	9,31,31',33,33'
D	2.0	1.00172	0.0	0.53205	6,6',9,9',31
E	2.63124	1.24730	0.0	0.49536	9,9',33,35
F	1.16425	1.33096	0.63179	0.44123	6,29,29',31,31'

Substitutionals		x	y	z	d	Touching
A	14	5.0	0.12082	0.0	1.01455	12,14',14'',16,41
B	9	2.50001	0.81250	0.5	1.01108	6,9',9'',35
C	20	7.43685	0.75176	0.5	1.00597	18,18',20',20'',22,22',44

5.3 DENSEST [111] BOUNDARIES

Listed in order of increasing angle.



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.28868	1.63299
3	-0.50000	-0.86603	0.00000
4	0.00000	-0.57735	0.81650
5	0.50000	-0.86603	0.00000
6	0.50000	-0.28868	1.63299
7	1.00000	-0.57735	0.81650
8	1.00000	0.00000	-0.00000
9	1.50000	-0.28868	1.63299
10	1.50000	0.28868	0.81650
11	2.00000	-0.00000	-0.00000
12	2.00000	0.57735	1.63299
13	2.50000	0.28868	0.81650
14	2.50000	0.86603	-0.00000
15	3.00000	0.57735	1.63299
16	3.00000	1.15470	0.81650
17	3.50000	0.86603	-0.00000
18	-0.94573	0.30079	0.12292
19	-0.38122	0.42185	0.93942
20	-0.76831	0.85021	-0.69357
21	-0.59089	1.39962	0.93942
22	-0.20380	0.97127	0.12292
23	-0.02638	1.52068	-0.69357
24	0.36072	1.09232	0.93942
25	0.53814	1.64174	0.12292
26	0.92523	1.21338	-0.69357
27	1.10265	1.76279	0.93942
28	1.48975	1.33444	0.12292
29	1.66717	1.88385	-0.69357
30	2.05427	1.45549	0.93942
31	2.23169	2.00491	0.12292
32	2.61878	1.57655	-0.69357
33	2.79620	2.12596	0.93942

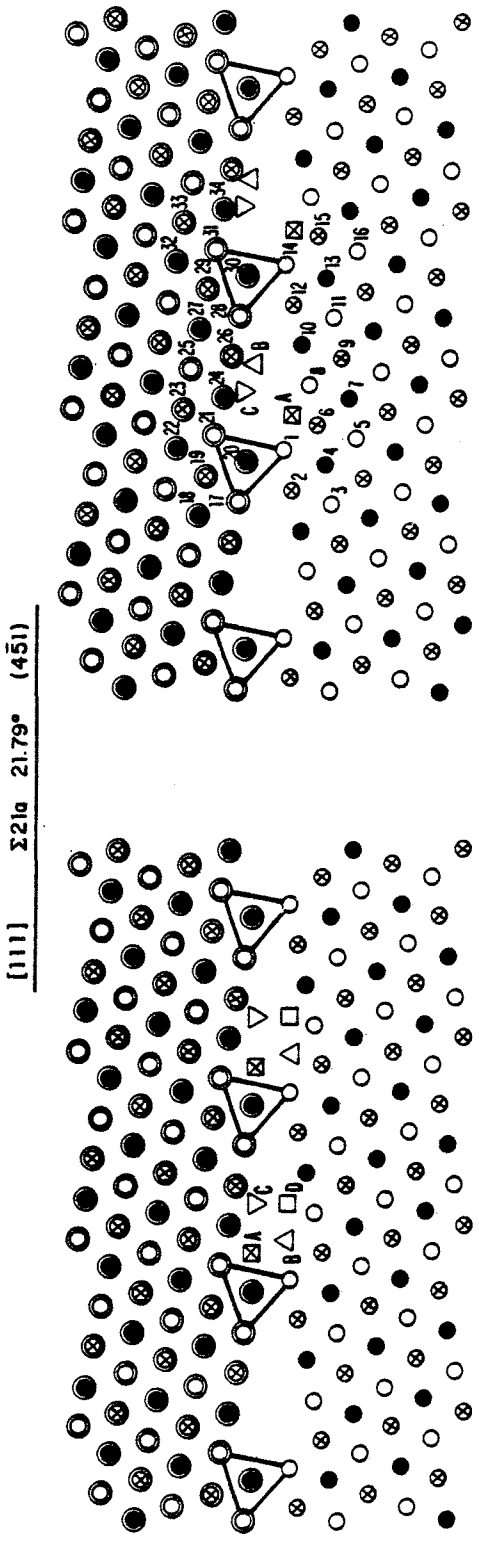
[111] $\Sigma 31a$ 17.90° $(5\bar{6}1)$ ΔZ = 0.12292

v^{EX} = 0.49482

Contacts: 1-18, 1-22, 2-19.

Interstitials	x	y	z	d	Touching
A	0.14325	0.58724	1.71721	0.89904	1,6,20,23
B	0.5	0.19769	0.75216	0.84914	1,4,7,8,24
C	0.79679	0.81563	0.23561	0.74592	8,24,25,28
D	1.0	0.39649	1.50511	0.71559	6,9,10,26
E	1.37145	0.65469	-0.30688	0.62576	8,12,26,28
F	1.39135	1.02972	1.12125	0.61717	10,26,27,30
G	1.92808	0.83961	0.50560	0.52765	10,14,28,30
H	1.98466	1.23996	2.00401	0.51914	12,28,29,32
I	2.49062	1.01129	1.31597	0.45534	12,16,30,32

Substitutionals		x	y	z	d	Touching
A	6	0.52337	0.16658	1.48635	1.17492	8,9,19,24
B	26	0.97142	0.83490	-0.66939	1.14099	8,12,24,28
C	24	0.58975	0.83887	0.81864	1.12723	10,19,22,25,26,27
D	10	1.28731	0.57957	0.84389	1.12660	8,12,24,28
E	8	1.0	0.32872	-0.11622	1.11808	1,6,9,10,11,26
F	28	1.50142	1.07947	0.15266	1.06497	10,14,26,30
G	12	1.84309	0.75781	1.66528	1.05740	10,14,26,30
H	30	2.02324	1.34234	0.97764	1.01517	12,16,28,32
I	14	2.40372	0.92117	0.03946	1.01306	11,12,13,16,28,32



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.28868	1.63299
3	-0.50000	-0.86603	-0.00000
4	-0.00000	-0.57735	0.81650
5	0.50000	-0.86603	-0.00000
6	0.50000	-0.28868	1.63299
7	1.00000	-0.57735	0.81650
8	1.00000	-0.00000	-0.00000
9	1.50000	-0.28868	1.63299
10	1.50000	0.28868	0.81650
11	2.00000	-0.00000	-0.00000
12	2.00000	0.57735	1.63299
13	2.50000	0.28868	0.81650
14	2.50000	0.86603	-0.00000
15	3.00000	0.57735	1.63299
16	3.00000	-0.00000	-0.00000
17	-0.92027	0.36060	0.15191
18	-1.27741	0.81423	0.96841
19	-0.70598	0.89671	-0.66459
20	-0.34884	0.44308	0.96841
21	-0.13456	0.97919	0.15191
22	-0.49170	1.43282	0.96841
23	0.07973	1.51530	-0.66459
24	0.43687	1.06167	0.96841
25	0.65116	1.59778	0.15191
26	1.00830	1.14415	-0.66459
27	1.22259	1.68026	0.96841
28	1.57973	1.22663	0.15191
29	1.79402	1.76274	-0.66459
30	2.15116	1.30910	0.96841
31	2.36544	1.84522	0.15191
32	2.00830	2.29885	0.96841
33	2.57973	2.38133	-0.66459
34	2.93687	1.92769	0.96841

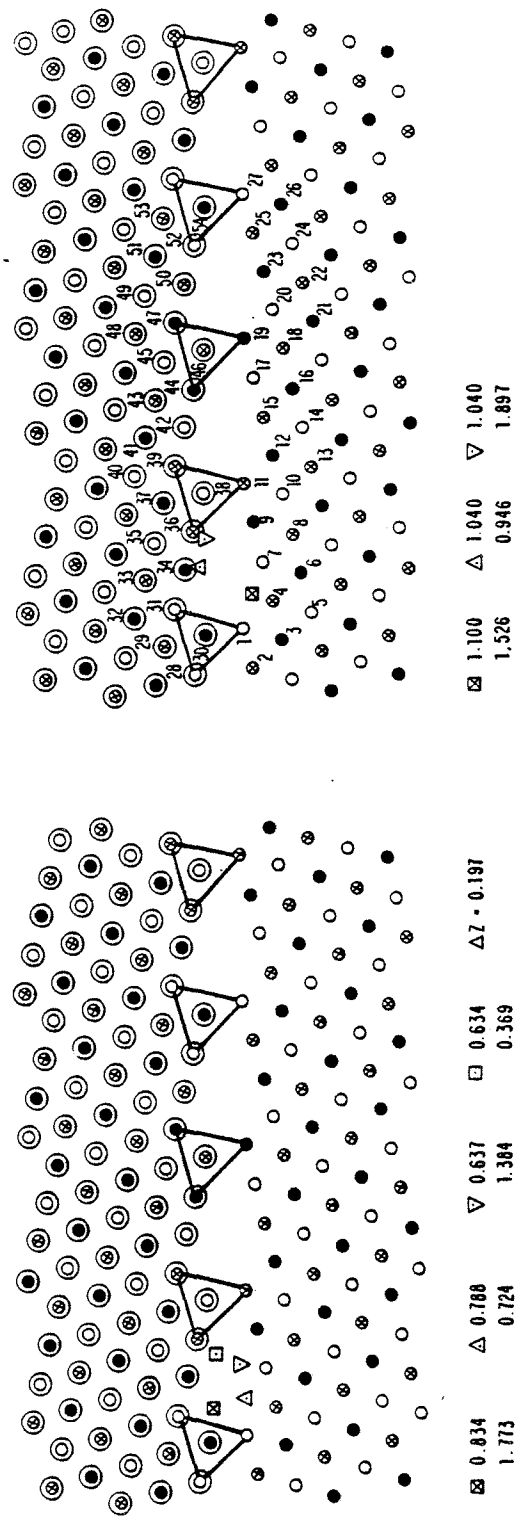
[111] $\Sigma 21a$ 21.79° $(4\bar{5}1)$ $\Delta z = -0.15191$

$$v^{EX} = 0.47564$$

Contacts: 1-17, 1-21, 2-20

Interstitials	x	y	z	d	Touching
A	0.17629	0.58437	1.73847	0.87416	1',6,19',23
B	0.50000	0.18120	0.74050	0.82337	1,4,7,8,24
C	0.86573	0.78744	0.28853	0.69865	8,24,25,28
D	1.00000	0.36453	1.48251	0.67250	6,9,10,26
E	1.42219	0.59565	2.16302	0.56860	8,12,26,28
F	1.47956	0.97602	1.18582	0.56110	10,26,27,30
G	1.99562	0.74557	0.52182	0.47135	10,14,28,30

Substitutionals		x	y	z	d	Touching
A	6	0.50000	0.07218	1.50542	1.14148	1,2,4,7,8,9,20
B	26	1.00296	0.83631	1.81974	1.09381	10,12,24,28
C	24	0.61337	0.83525	0.86776	1.09049	10,20,21,26
D	10	1.26109	0.42660	0.91403	1.08385	7,8,9,12,24
E	8	1.00000	0.27221	2.35325	1.08169	1,6,9,10,11,26
F	28	1.52616	1.09260	0.20294	1.02331	10,25,26,27,30
G	12	1.88131	0.64587	1.68145	1.02101	9,10,11,14,26,30



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.28868	1.63299
3	-0.00000	-0.57735	0.81650
4	0.50000	-0.28868	1.63299
5	0.50000	-0.86603	0.00000
6	1.00000	-0.57735	0.81650
7	1.00000	0.00000	0.00000
8	1.50000	-0.28868	1.63299
9	1.50000	0.28868	0.81650
10	2.00000	-0.00000	-0.00000
11	2.00000	0.57735	1.63299
12	2.50000	0.28868	0.81650
13	2.50000	-0.28868	1.63299
14	3.00000	-0.00000	-0.00000
15	3.00000	0.57735	1.63299
16	3.50000	0.28868	0.81650
17	3.50000	0.86603	-0.00000
18	4.00000	0.57735	1.63299
19	4.00000	1.15470	0.81650
20	4.50000	0.86603	-0.00000
21	4.50000	0.28868	0.81650
22	5.00000	0.57735	1.63299
23	5.00000	1.15470	0.81650
24	5.50000	0.86603	-0.00000
25	5.50000	1.44338	1.63299
26	6.00000	1.15470	0.81650
27	6.00000	1.73205	-0.00000
28	-0.87251	0.44710	0.19707
29	-0.60328	0.95783	-0.61942
30	-0.29558	0.46930	1.01357
31	-0.02635	0.98003	0.19707
32	-0.33405	1.46856	1.01357
33	0.24288	1.49077	-0.61942
34	0.55057	1.00224	1.01357
35	0.81980	1.51297	0.19707
36	1.12749	1.02445	-0.61942
37	1.39672	1.53518	1.01357
38	1.70442	1.04665	0.19707
39	1.97365	1.55738	-0.61942
40	1.66596	2.04591	0.19707
41	2.24288	2.06812	1.01357
42	2.55057	1.57959	0.19707
43	2.81980	2.09032	-0.61942
44	3.12749	1.60180	1.01357
45	3.39672	2.11253	0.19707
46	3.70442	1.62400	-0.61942
47	3.97365	2.13473	1.01357
48	3.66596	2.62326	-0.61942
49	4.24288	2.64547	0.19707
50	4.55057	2.15694	-0.61942
51	4.81980	2.66767	1.01357
52	5.12749	2.17915	0.19707
53	5.39672	2.68988	-0.61943
54	5.70442	2.20135	1.01357

[111] Σ13b 27.80° $(3\bar{4}1)$ $\Delta z = 0.19707$

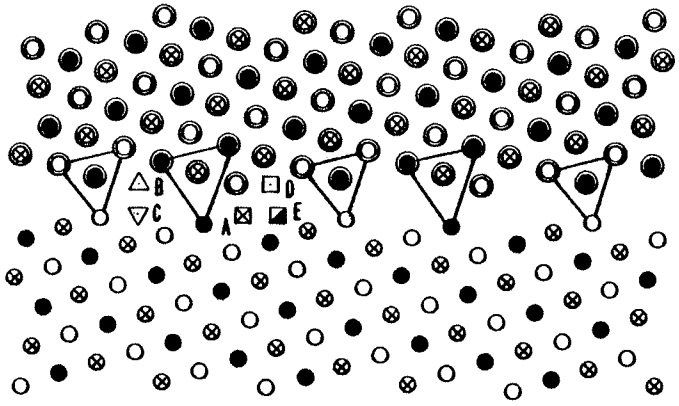
$v^{EX} = 0.44247$

Contacts: 1-28, 1-31, 2-30

Interstitials	x	y	z	d	Touching
A	0.22829	0.57573	1.77336	0.83383	1,4,29,33
B	0.5	0.15795	0.72406	0.78797	1,3,6,7,34
C	0.91643	0.37083	1.38443	0.63726	4,9,34,36
D	0.97155	0.72862	0.36886	0.63432	7,34,35,38
E	1.5	0.49057	-0.25574	0.49139	7,10,36,38
F	1.48410	0.86429	1.23510	0.42381	9,11,36,37

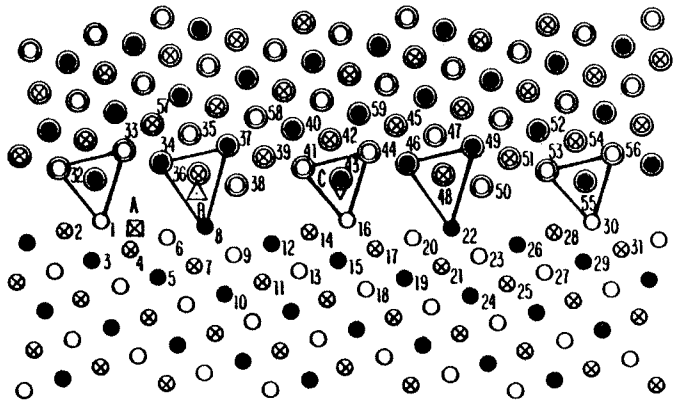
Substitutionals		x	y	z	d	Touching
A	4	0.5	0.01387	1.52603	1.10045	1,2,3,6,7,8,30
B	34	0.65211	0.84103	0.94621	1.04042	9,30,31,35,36,37
C	36	1.03904	0.85665	-0.55236	1.04008	7,33,34,35,38
D	7	1.0	0.18072	-0.06389	1.03641	1,4,8,9,10,36
E	9	1.34415	0.37866	0.88012	1.03611	6,7,8,11,34

[111] Σ39a 32.21° (5$\bar{7}$2)



⊠ 0.890 △ 0.823 ▽ 0.769 ⊡ 0.718 ◪ 0.664 △ Z = 0.152

1.603 1.890 0.732 1.029 -0.137



⊠ 1.109 △ 1.077 ▽ 1.061

1.522 1.749 0.990

[111] $\Sigma 39a$ 32.21° $(5\bar{7}2)$ Δz = 0.15188

v^{EX} = 0.47914

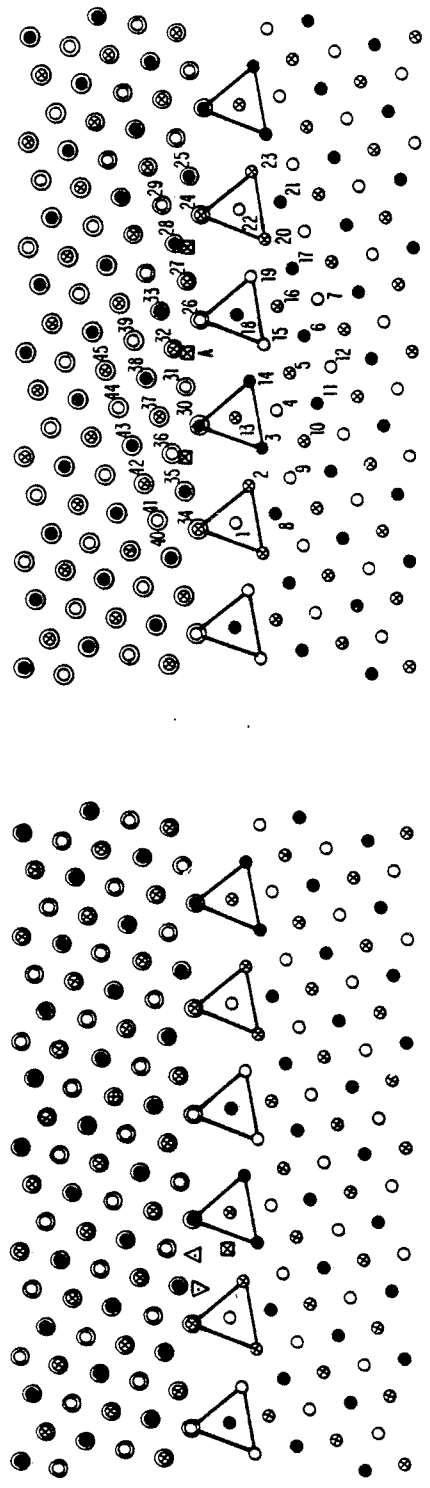
Contracts: 8-38, 9-38, 16-41

Interstitials	x	y	z	d	Touching
A	2.03716	0.53437	1.60261	0.88950	11,12,36,39
B	0.42288	0.58264	1.89008	0.82344	1,4,33,36
C	0.53370	0.16979	0.73243	0.76943	5,6,32,34
D	2.30531	1.09792	1.02856	0.71784	12,37,39,40
E	2.52952	0.67258	-0.13679	0.66425	13,14,38,41
F	0.91592	0.36159	1.37743	0.62422	4,8,34,36
G	1.04099	0.72707	0.33022	0.59919	6,8,34,35
H	2.96706	0.84050	0.55398	0.53827	12,16,41,43
I	2.77785	1.27374	1.50621	0.48375	14,39,42,43
J	1.5	0.34266	2.02215	0.48329	6,7,9,36
K	3.04383	1.21898	1.99167	0.47278	14,16,41,42

Substitutionals		x	y	z	d	Touching
A	4	0.5	0.02638	1.52161	1.10871	1,2,3,5,6,7,32
B	36	1.27069	0.71733	1.74926	1.07669	6,7,34,38
C	43	3.28181	1.33185	0.99049	1.06058	14,41,42,46
D	39	2.22427	1.25165	1.70238	1.06034	14,36,37,38,40,41,42
E	14	2.80031	0.69264	1.71452	1.05894	11,12,13,16,39
F	12	2.5	0.49857	0.74229	1.04896	8,9,13,14,15,38
G	6	1.0	0.19505	-0.06896	1.04235	1,4,7,8,9,36
H	8	1.41444	0.35405	0.85425	1.02668	6,7,34,38
I	34	0.71060	0.90642	0.92541	1.01654	8,32,33,35,36,37
J	44	3.60260	1.85361	0.13247	1.00339	16,41,42,43,45,46,47

[111] Σ39a 32.21° ($5\bar{7}2$) $\Delta Z = 0.15188$

	X	Y	Z		X	Y	Z
1	0.00000	0.00000	0.00000	31	7.50000	1.44338	1.63299
2	-0.50000	-0.28868	1.63299	32	-0.23069	0.54762	0.96837
3	-0.00000	-0.57735	0.81650	33	0.07701	1.03615	0.15188
4	0.50000	-0.28868	1.63299	34	0.65393	1.01394	0.96837
5	1.00000	-0.57735	0.81650	35	0.96162	1.50247	0.15188
6	1.00000	0.00000	-0.00000	36	1.23085	0.99173	-0.66462
7	1.50000	-0.28868	1.63299	37	1.53854	1.48026	0.96837
8	1.50000	0.28868	0.81650	38	1.80777	0.96953	0.15188
9	2.00000	-0.00000	-0.00000	39	2.11547	1.45805	-0.66462
10	2.00000	-0.57735	0.81650	40	2.42316	1.94658	0.96837
11	2.50000	-0.28868	1.63299	41	2.69239	1.43585	0.15188
12	2.50000	0.28868	0.81650	42	3.00008	1.92438	-0.66462
13	3.00000	-0.00000	-0.00000	43	3.26931	1.41364	0.96837
14	3.00000	0.57735	1.63299	44	3.57701	1.90217	0.15188
15	3.50000	0.28868	0.81650	45	3.88470	2.39070	-0.66462
16	3.50000	0.86603	-0.00000	46	4.15393	1.87996	0.96837
17	4.00000	0.57735	1.63299	47	4.46162	2.36849	0.15188
18	4.00000	-0.00000	-0.00000	48	4.73085	1.85776	-0.66462
19	4.50000	0.28868	0.81650	49	5.03854	2.34629	0.96837
20	4.50000	0.86603	-0.00000	50	5.30777	1.83555	0.15188
21	5.00000	0.57735	1.63299	51	5.61547	2.32408	-0.66462
22	5.00000	1.15470	0.81650	52	5.92316	2.81261	0.96837
23	5.50000	0.86603	-0.00000	53	6.19239	2.30187	0.15188
24	5.50000	0.28868	0.81650	54	6.50008	2.79040	-0.66462
25	6.00000	0.57735	1.63299	55	6.76931	2.27967	0.96837
26	6.00000	1.15470	0.81650	56	7.07701	2.76819	0.15188
27	6.50000	0.86603	-0.00000	57	0.38470	1.52468	-0.66462
28	6.50000	1.44338	1.63299	58	1.84624	1.96879	0.15188
29	7.00000	1.15470	0.81650	59	3.30778	2.41290	0.96837
30	7.00000	1.73205	-0.00000				



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	0.28867	1.63299
3	1.00000	0.57735	0.81650
4	1.50000	0.86603	0.00000
5	2.00000	1.15470	1.63299
6	2.50000	1.44338	0.81650
7	3.00000	1.73205	0.00000
8	0.50000	-0.28867	0.81650
9	1.00000	0.00000	0.00000
10	1.50000	0.28868	1.63299
11	2.00000	0.57735	0.81650
12	2.50000	0.86603	0.00000
13	1.00000	1.15470	1.63299
14	1.50000	1.44338	0.81650
15	2.00000	1.73205	0.00000
16	2.50000	2.02073	1.63299
17	3.00000	2.30940	0.81650
18	2.00000	2.30940	0.81650
19	2.50000	2.59808	0.00000
20	3.00000	2.88675	1.63299
21	3.50000	3.17543	0.81650
22	3.00000	3.46410	0.00000
23	3.50000	3.75278	1.63299
24	2.53843	3.73060	1.35934
25	2.75271	4.26671	0.54285
26	1.53843	2.57590	-0.27365
27	1.75272	3.11201	1.35934
28	1.96700	3.64812	0.54285
29	2.18128	4.18423	-0.27365
30	0.53843	1.42120	0.54285
31	0.75271	1.95731	-0.27365
32	0.96700	2.49343	1.35934
33	1.18129	3.02953	0.54285
34	-0.46158	0.26650	1.35934
35	-0.24728	0.80261	0.54285
36	-0.03300	1.33872	-0.27365
37	0.18129	1.87483	1.35934
38	0.39557	2.41094	0.54285
39	0.60986	2.94705	-0.27365
40	-1.03301	0.18402	0.54285
41	-0.81871	0.72013	-0.27365
42	-0.60443	1.25624	1.35934
43	-0.39014	1.79235	0.54285
44	-0.17586	2.32846	-0.27365
45	0.03843	2.86458	1.35934

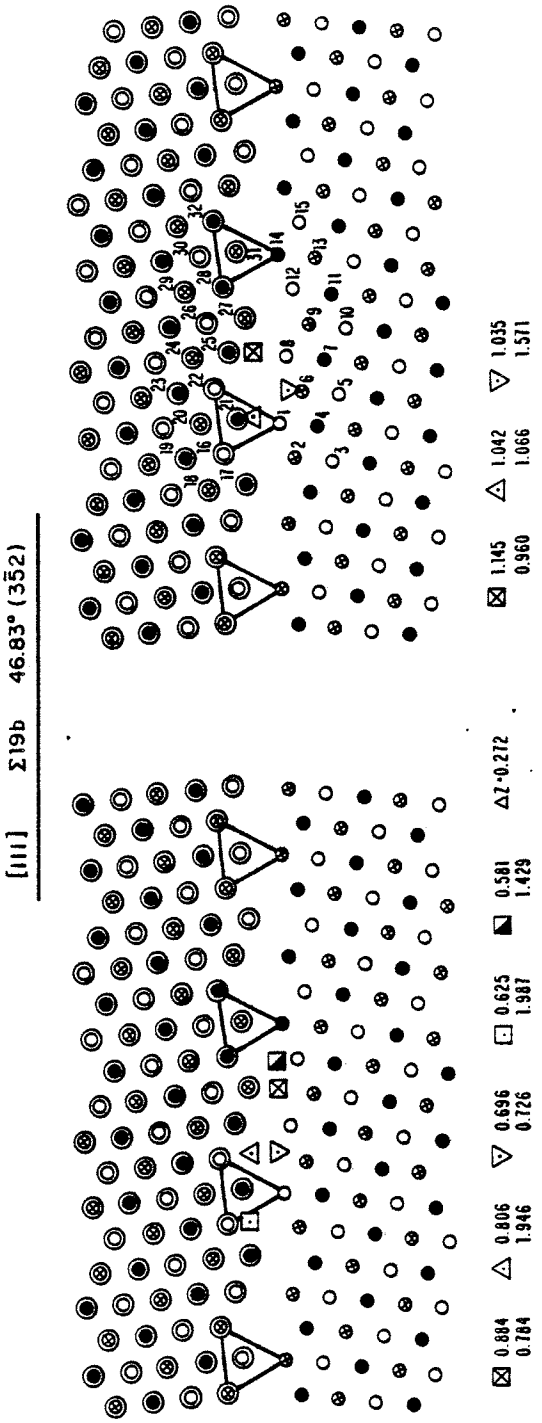
[111] $\Sigma 7$ 38.21° $(2\bar{3}1)$ $\Delta Z = -0.27365$

$$V^{EX} = 0.37534$$

Contacts: 1-35, 2-34, 3-30

Interstitials	x	y	z	d	Touching
A	0.62581	0.79337	-0.06726	0.75956	4,9,30,36
B	0.22239	1.01432	1.24304	0.73861	2,30,35,37,42
C	-0.08985	0.60265	1.99516	0.52010	1,2,36,41
D	0.27307	0.41969	0.92798	0.50427	2,3,8,35

Substitutionals		x	y	z	d	Touching
A	32	1.09244	2.33409	1.28765	1.04574	18,26,27,31,33,37,38



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.28868	1.63299
3	-0.50000	-0.86603	-0.00000
4	-0.00000	-0.57735	0.81650
5	0.50000	-0.86603	-0.00000
6	0.50000	-0.28868	1.63299
7	1.00000	-0.57735	0.81650
8	1.00000	-0.00000	-0.00000
9	1.50000	-0.28868	1.63299
10	1.50000	-0.86603	-0.00000
11	2.00000	-0.57735	0.81650
12	2.00000	-0.00000	-0.00000
13	2.50000	-0.28868	1.63299
14	2.50000	0.28868	0.81650
15	3.00000	-0.00000	-0.00000
16	-0.57895	0.77993	0.27217
17	-1.00000	0.38490	1.08867
18	-1.13158	0.94706	-0.54433
19	-0.71053	1.34209	1.08867
20	-0.15790	1.17496	-0.54433
21	-0.02632	0.61280	1.08867
22	0.39473	1.00783	0.27217
23	0.26315	1.56999	1.08867
24	0.81579	1.40286	-0.54433
25	0.94737	0.84070	1.08867
26	1.36842	1.23573	0.27217
27	1.50000	0.67358	-0.54433
28	1.92105	1.06861	1.08867
29	1.78947	1.63076	-0.54433
30	2.34210	1.46364	0.27217
31	2.47368	0.90148	-0.54433
32	2.89473	1.29651	1.08867

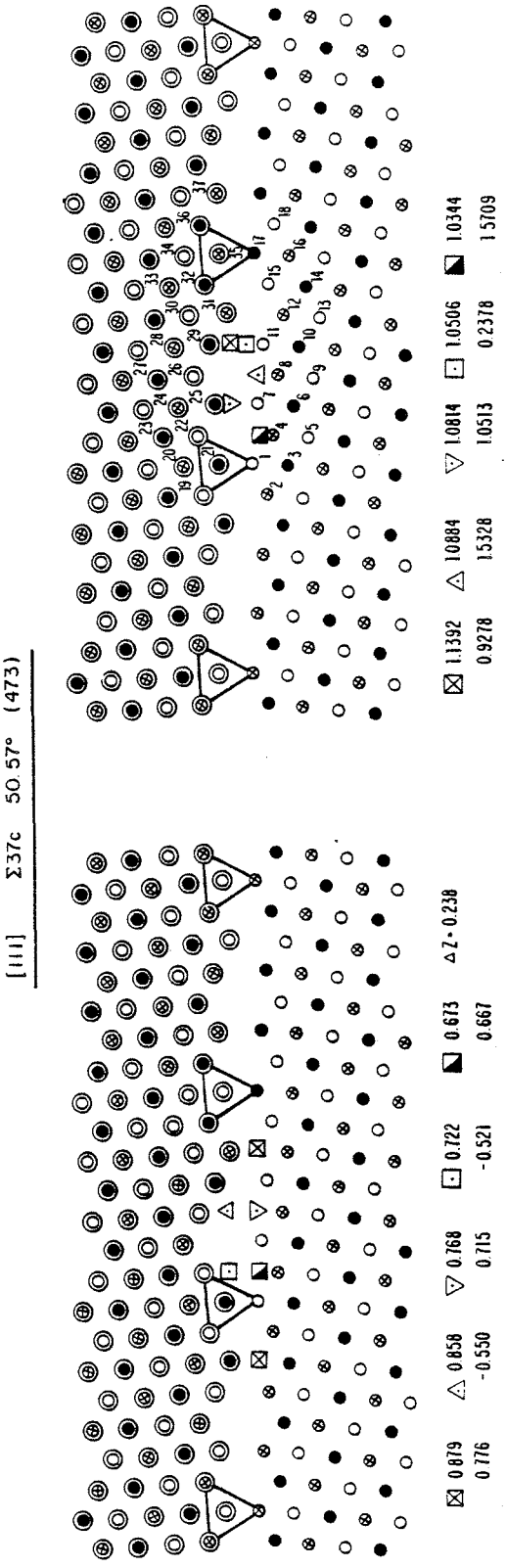
[111] $\Sigma 19b$ 46.83° $(3\bar{5}2)$ $\Delta z = 0.27217$

$v^{EX} = 0.42918$

Contacts: 8-27, 12-27, 9-27'

Interstitials	x	y	z	d	Touching
A	1.57965	0.24269	0.78398	0.84415	11,12,14,25
B	0.50000	0.55810	1.94598	0.80555	1,6,8,20,22,24
C	0.59295	0.16099	0.72621	0.69587	7,8,21,25
D	-0.50000	0.44263	1.98681	0.62481	1,2,16,18,20
E	2.00000	0.28867	1.42887	0.58114	9,13,14,27
F	-1.00000	0.08627	1.19425	0.52720	6,7,9,25
G	1.50000	0.51459	0.17750	0.47826	8,12,26,27
H	1.00000	0.61584	0.39465	0.46288	8,22,25,26
I	0.97540	0.72090	-0.04908	0.44598	8,22,26,27
J	1.00000	0.19245	1.76907	0.41421	6,8,9,27

Substitutionals		x	y	z	d	Touching
A	25	1.03061	0.48505	0.95953	1.14485	7,21,22,26,27,28
B	21	0.02055	0.41258	1.06630	1.04234	4,6,17,25
C	6	0.50000	-0.11226	1.57062	1.03471	1,2,4,7,8,9,21
D	22	0.42307	0.88675	0.22820	1.01732	1,16,20,21,24,25,26
E	8	0.97451	0.19132	0.16650	1.01395	1,7,22,27
F	1	-0.00217	0.00625	0.00177	1.00438	2,4,8,16
G	28	1.92308	1.05996	1.08552	1.00008	14,25,26,27,30,31,32



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.28868	1.63299
3	-0.00000	-0.57735	0.81650
4	0.50000	-0.28868	1.63299
5	0.50000	-0.86603	0.00000
6	1.00000	-0.57735	0.81650
7	1.00000	0.00000	0.00000
8	1.50000	-0.28868	1.63299
9	1.50000	-0.86603	0.00000
10	2.00000	-0.57735	0.81650
11	2.00000	0.00000	0.00000
12	2.50000	-0.28868	1.63299
13	2.50000	-0.86603	0.00000
14	3.00000	-0.57735	0.81650
15	3.00000	-0.00000	0.00000
16	3.50000	-0.28868	1.63299
17	3.50000	0.28868	0.81650
18	4.00000	-0.00000	-0.00000
19	-0.60575	0.75929	0.23778
20	-0.15980	1.12599	-0.57872
21	-0.06521	0.55644	1.05428
22	0.38074	0.92313	0.23778
23	0.28614	1.49268	1.05428
24	0.82668	1.28983	-0.57872
25	0.92128	0.72028	1.05428
26	1.36722	1.08698	0.23778
27	1.27263	1.65652	1.05428
28	1.81317	1.45367	-0.57872
29	1.90776	0.88412	1.05428
30	2.35371	1.25082	0.23778
31	2.44830	0.68127	-0.57872
32	2.89425	1.04797	1.05428
33	2.79966	1.61751	-0.57872
34	3.34020	1.41466	0.23778
35	3.43479	0.84511	-0.57872
36	3.88074	1.21181	1.05428
37	4.42128	1.00895	-0.57872

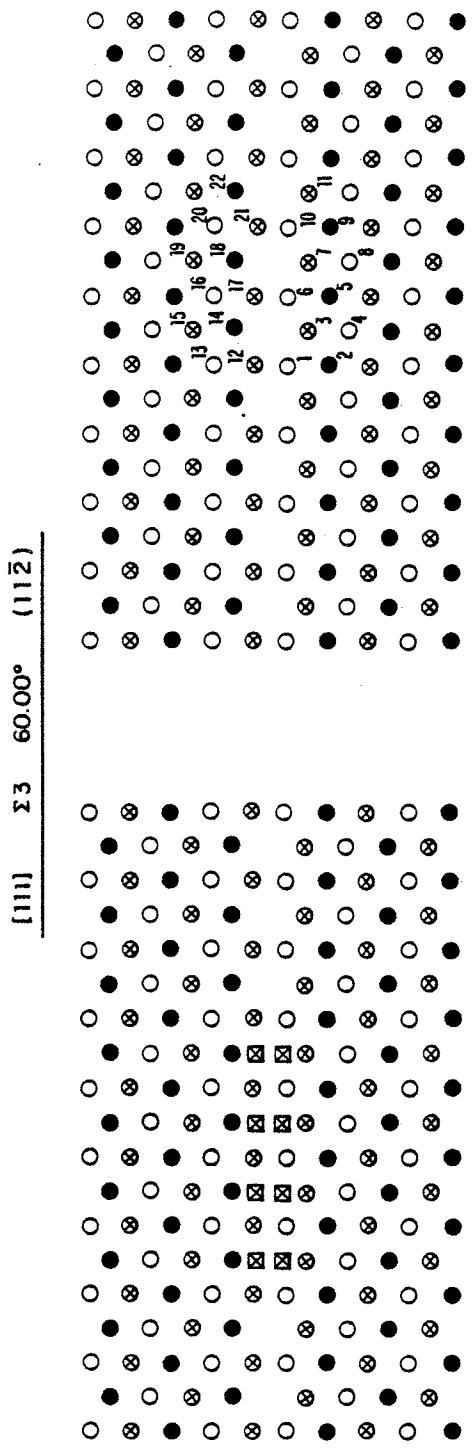
[111] $\Sigma 37c$ 50.57° $(4\bar{7}3)$ $\Delta z = 0.23778$

$V^{EX} = 0.44395$

Contacts: 1-19, 11-31, 12-31

Interstitials	x	y	z	d	Touching
A	2.52308	0.23107	0.77577	0.87900	14,15,29,32
B	1.44813	0.59982	-0.55003	0.85810	7,8,24,28
C	1.5	0.14464	0.71464	0.76820	6,7,10,11,25
D	0.44792	0.51862	-0.52144	0.72221	1,4,20,24
E	0.5	0.07657	0.66651	0.67344	1,3,6,7,21
F	2.94774	0.72591	0.32649	0.59533	15,30,32,34
G	3.0	0.30132	1.43781	0.59523	12,16,17,31
H	2.0	0.24577	1.44699	0.51027	8,12,29,31
I	1.94745	0.64516	0.35626	0.47772	11,26,29,30
J	1.0	0.02227	1.21687	0.44201	4,6,8,25

Substitutionals		x	y	z	d	Touching
A	29	1.96639	0.53116	0.92777	1.13918	11,25,26,30,31,32
B	8	1.5	-0.00529	1.53280	1.08839	4,6,7,10,11,12,25
C	25	0.96849	0.43602	1.05129	1.08138	4,6,21,29
D	11	1.98520	0.26886	0.23778	1.05057	10,26,29,31
E	4	0.5	-0.11311	1.57092	1.03438	1,2,3,6,7,8,21
F	7	1.0	0.17412	-0.06157	1.03382	1,4,8,11,22
G	26	1.39509	0.91918	0.17764	1.03229	7,22,24,25,28,29,30
H	35	3.46001	0.69324	-0.57578	1.02358	15,16,31,37
I	15	3.0	0.05837	-0.02063	1.00383	11,12,16,17,18,31
J	22	0.38545	0.89474	0.22760	1.00093	1,19,20,21,24,25,26



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.00000	-0.57735	0.81650
3	0.50000	-0.28868	1.63299
4	0.50000	-0.86603	0.00000
5	1.00000	-0.57735	0.81650
6	1.00000	0.00000	0.00000
7	1.50000	-0.28868	1.63299
8	1.50000	-0.86603	0.00000
9	2.00000	-0.57735	0.81650
10	2.00000	-0.00000	0.00000
11	2.50000	-0.28868	1.63299
12	0.00000	0.47509	1.22475
13	-0.00000	1.05244	-0.40825
14	0.50000	0.76376	0.40825
15	0.50000	1.34111	1.22475
16	1.00000	1.05244	-0.40825
17	1.00000	0.47509	1.22475
18	1.50000	0.76376	0.40825
19	1.50000	1.34111	1.22475
20	2.00000	1.05244	-0.40825
21	2.00000	0.47509	1.22475
22	2.50000	0.76376	0.40825

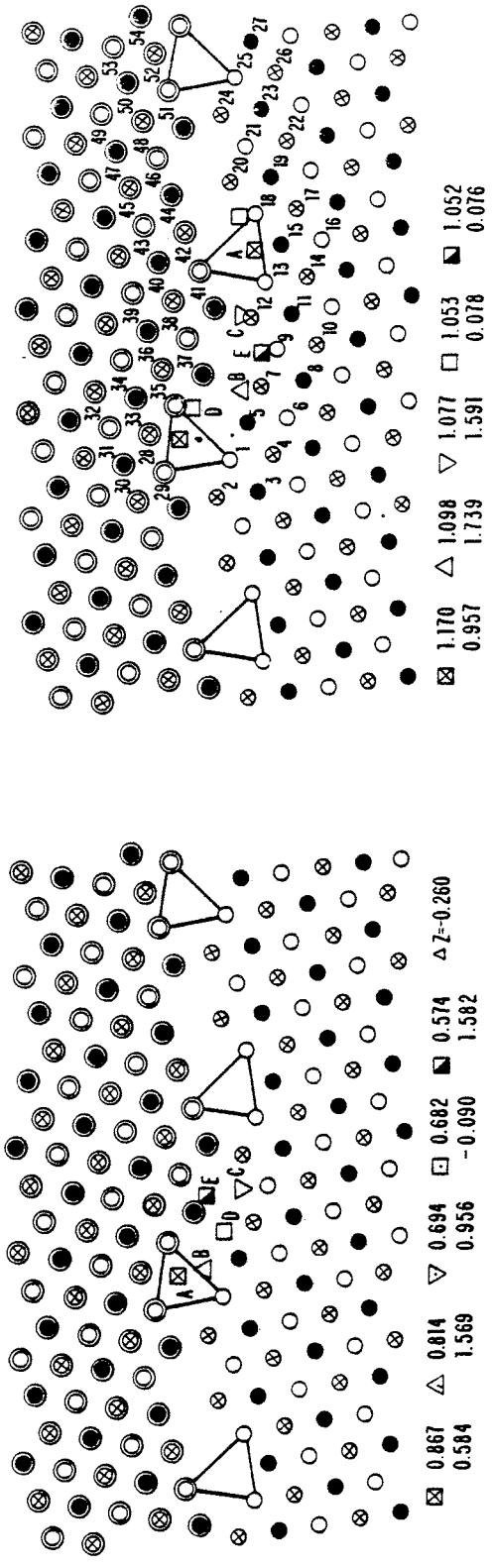
[111] $\Sigma 3$ 60.00° $(11\bar{2})$ $\Delta z = -0.40825$

$v^{EX} = 0.20924$

Contacts: 1-14, 6-14, 3-12, 3-17

Interstitials	x	y	z	d	Touching
A	0.50000	0.04715	0.76727	0.60303	2,5,12,14,17

Substitutionals	x	y	z	d	Touching
none > 1.0000					



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.28868	1.63299
3	-0.00000	-0.57735	0.81650
4	0.50000	-0.28868	1.63299
5	0.50000	0.28868	0.81650
6	1.00000	0.00000	-0.00000
7	1.00000	0.57735	1.63299
8	1.50000	0.28868	0.81650
9	1.50000	0.86603	-0.00000
10	2.00000	0.57735	1.63299
11	2.00000	1.15470	0.81650
12	1.50000	1.44338	1.63299
13	2.00000	1.73205	-0.00000
14	2.50000	1.44338	1.63299
15	2.50000	2.02073	0.81650
16	3.00000	1.73205	-0.00000
17	3.00000	2.30940	1.63299
18	2.50000	2.59808	-0.00000
19	3.00000	2.88675	0.81650
20	2.50000	3.17543	1.63299
21	3.00000	3.46410	-0.00000
22	3.50000	3.17543	1.63299
23	3.50000	3.75278	0.81650
24	3.00000	4.04145	1.63299
25	3.50000	4.33013	-0.00000
26	4.00000	4.04145	1.63299
27	4.00000	4.61880	0.81650
28	-0.85669	0.46165	-0.25974
29	-1.03411	-0.08776	0.55676
30	-1.42121	0.34060	1.37326
31	-1.24379	0.89001	0.55676
32	-1.06637	1.43942	-0.25974
33	-0.67927	1.01107	1.37326
34	-0.50185	1.56048	0.55676
35	-0.11476	1.13212	-0.25974
36	0.06266	1.68154	1.37325
37	0.44976	1.25318	0.55676
38	0.62718	1.80260	-0.25974
39	0.24008	2.23095	0.55676
40	0.80460	2.35201	1.37325
41	1.19169	1.92365	0.55676
42	1.36911	2.47307	-0.25974
43	0.98202	2.90142	0.55676
44	1.54653	3.02248	1.37325
45	1.15944	3.45084	-0.25974
46	1.72395	3.57189	0.55676
47	1.33686	4.00025	1.37326
48	1.90137	4.12131	-0.25974
49	1.51428	4.54966	0.55676
50	2.07879	4.67072	1.37326
51	2.46589	4.24236	0.55676
52	2.64331	4.79178	-0.25974
53	2.25621	5.22014	0.55676
54	2.82073	5.34119	1.37326

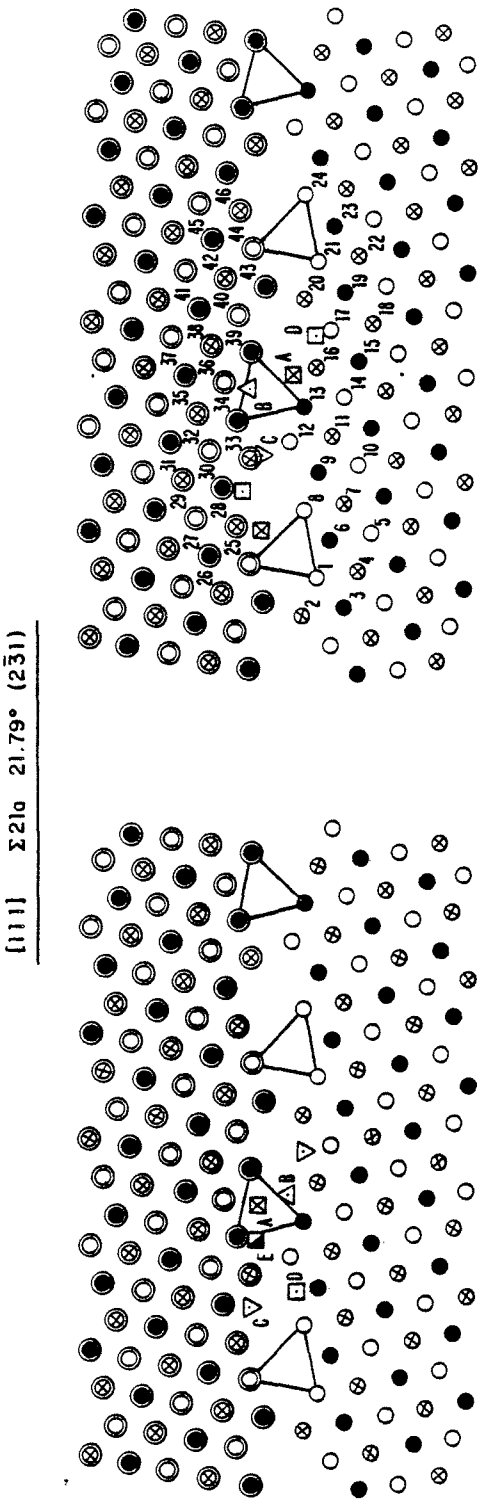
[111] $\Sigma 31a$ 17.90° $(4\bar{1}\bar{1}7)$ ΔZ = - 0.25974

V^{EX} = 0.49153

Contacts: 2-28, 5-37, 13-41, 20-44.

Interstitials	x	y	z	d	Touching
A	-0.34473	0.64086	0.58448	0.86671	1,31,33,34
B	0.03495	0.48751	1.56945	0.81414	4,5,33,35
C	1.17043	1.05631	0.95565	0.69379	7,8,11,12,37
D	0.60916	0.73928	-0.08963	0.68205	6,7,35,37
E	0.72578	1.31302	1.58179	0.57357	7,12,35,38
F	-0.68844	0.27547	1.14246	0.54193	2,29,30,33
G	1.29209	1.56342	-0.07162	0.46247	9,13,38,41
H	0.96909	1.17255	2.05386	0.45923	7,9,12,38

Substitutionals		x	y	z	d	Touching
A	15	2.15601	2.21933	0.95693	1.17024	11,13,14,17,18,19,41
B	7	0.74120	0.72678	1.73865	1.09806	4,5,6,9,12,35
C	12	1.44074	1.56082	1.59147	1.07681	11,13,38,39
D	18	2.31001	2.70777	0.07756	1.05343	13,15,19,20,21,42
E	9	1.31251	0.97427	0.07654	1.05205	6,7,8,11,12,13,37
F	5	0.08166	0.42123	1.02581	1.04709	3,4,33,37



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.28868	1.63299
3	-0.00000	-0.57735	0.81650
4	0.50000	-0.28868	1.63299
5	1.00000	0.00000	0.00000
6	0.50000	0.28868	0.81650
7	1.00000	0.57735	1.63299
8	0.50000	0.86603	0.00000
9	1.00000	1.15470	0.81650
10	1.50000	0.86603	0.00000
11	1.50000	1.44338	1.63299
12	1.00000	1.73205	0.00000
13	1.50000	2.02073	0.81650
14	2.00000	1.73205	0.00000
15	2.50000	2.02073	0.81650
16	2.00000	2.30940	1.63299
17	2.50000	2.59808	0.00000
18	3.00000	2.30940	1.63299
19	3.00000	2.88675	0.81650
20	2.50000	3.17543	1.63299
21	3.00000	3.46410	0.00000
22	3.50000	3.17543	1.63299
23	3.50000	3.75278	0.81650
24	3.50000	4.33013	0.00000
25	-0.57061	0.78284	-0.24811
26	-1.14204	0.70036	1.38488
27	-0.92776	1.23647	0.56838
28	-0.35633	1.31895	1.38488
29	-0.71347	1.77258	-0.24812
30	-0.14204	1.85506	0.56838
31	-0.49918	2.30870	1.38488
32	0.07224	2.39117	-0.24811
33	0.42939	1.93754	1.38488
34	0.64367	2.47365	0.56838
35	0.28653	2.92728	1.38488
36	0.85796	3.00976	-0.24811
37	0.50082	3.46340	0.56838
38	1.07224	3.54587	1.38488
39	1.42939	3.09224	0.56838
40	1.64367	3.62835	-0.24811
41	1.28653	4.08199	0.56838
42	1.85796	4.16446	1.38488
43	2.21510	3.71083	0.56838
44	2.42939	4.24694	-0.24811
45	2.07224	4.70058	0.56838
46	2.64367	4.78305	1.38488

[111] $\Sigma 21a$ 21.79° $(2\bar{3}1)$ $\Delta Z = -0.24811$

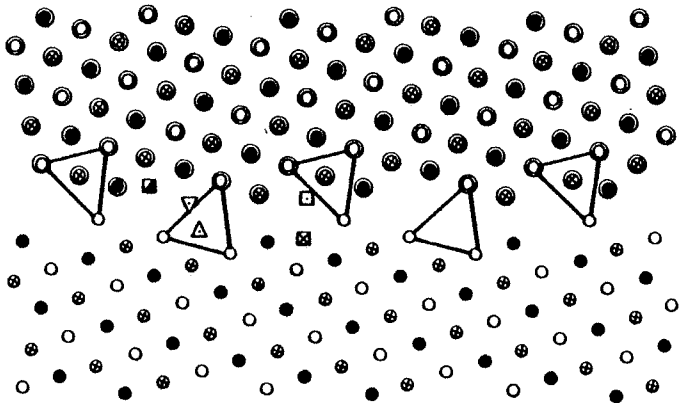
$$v^{EX} = 0.49375$$

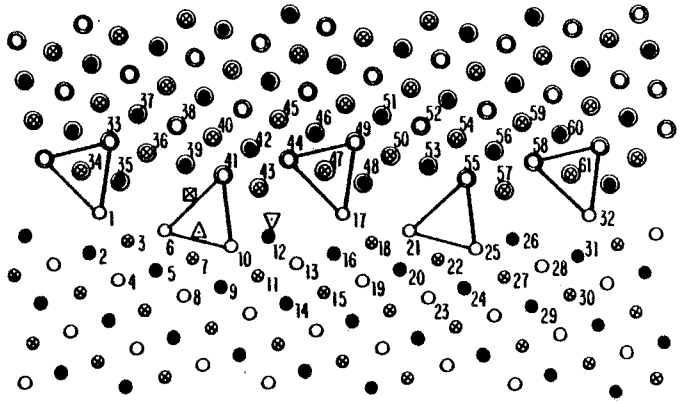
Contacts: 1-25, 13-34, 12-34.

Interstitials	x	y	z	d	Touching
A	1.15764	2.62911	1.41773	0.84262	13,35,36,38
B	1.55679	2.49509	-0.07283	0.77084	14,16,36,39
C	2.15081	2.79968	0.93963	0.72495	15,16,19,20,39
D	0.72113	1.31571	-0.63595	0.61931	7,8,11,12,33
E	0.79200	2.28524	-0,48680	0.53134	12,32,33,36
F	0.58771	1.73644	0.61548	0.48165	9,12,30,34

Substitutionals		x	y	z	d	Touching
A	28	-0.13185	1.03383	1.25658	1.14303	6,25,26,27,30,33
B	36	1.07799	2.73028	-0.37387	1.13760	12,32,34,35,38,39,40
C	33	0.57227	1.88593	1.43227	1.09459	9,11,32,34
D	30	0.01842	1.65124	0.47667	1.07432	8,27,28,29,32,33,34
E	8	0.38349	0.93329	0.04757	1.02026	1,6,9,12,25
F	9	0.89579	1.21487	0.85904	1.01622	6,7,8,11,12,13,33
G	12	0.86234	1.78958	-0.12793	1.00060	8,11,32,34

[111] Σ13b 27.80° (5$\bar{7}$2)





⊠ 0.826 1.558 △ 0.812 0.735 ▽ 0.784 1.784 ⊡ 0.701 0.738 ◪ 0.625 0.234 △Z = 0.057

⊠ 1.186 1.021 △ 1.167 1.494 ▽ 1.090 0.754

[111] Σ13b 27.80° $(5\bar{7}2)$ $\Delta Z = 0.05696$

$V^{EX} = 0.48069$

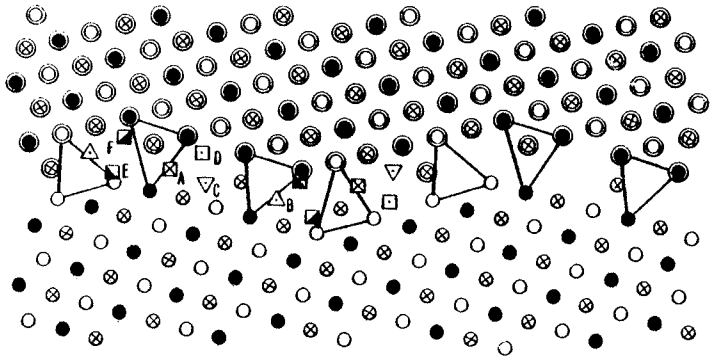
Contacts: 10-41, 17-47, 17-49

Interstitials	x	y	z	d	Touching
A	3.0	0.47156	1.55820	0.82600	11,12,15,16,47
B	1.5	0.17389	0.73533	0.81212	5,6,9,10,39
C	1.25789	0.55615	1.78446	0.78359	7,36,40,41
D	2.88367	1.04386	0.73823	0.70132	12,44,46,48
E	0.62629	0.68209	0.23441	0.62462	6,33,35,38,39
F	2.5	0.61126	2.36640	0.58813	10,13,43,44
G	0.79458	0.36284	1.32059	0.56057	3,35,36,39
H	2.000	0.23550	1.38989	0.52554	7,11,12,43
I	0.5	-0.09677	0.54395	0.49029	1,2,5,6,35
J	2.22166	0.87232	0.47797	0.45975	12,41,42,44
K	0.5	0.32476	-0.42101	0.45975	1,3,6,36

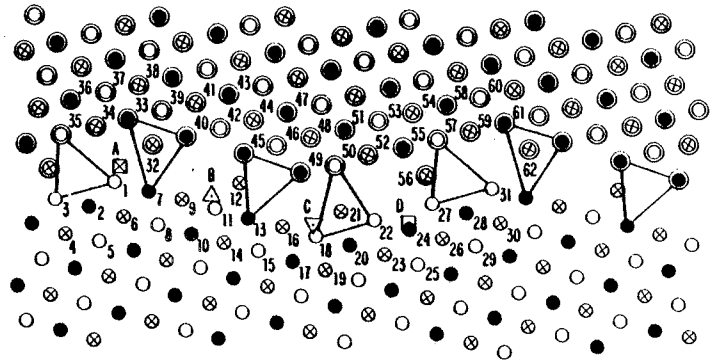
Substitutionals		x	y	z	d	Touching
A	39	1.24515	0.58032	1.02067	1.18636	7,35,36,40,41,42
B	7	1.5	0.10487	1.49386	1.16724	3,5,6,9,10,11,43
C	12	2.48661	0.53532	0.75390	1.08970	10,16,42,43
D	36	0.59850	0.73480	-0.66519	1.07857	3,33,34,35,38,39,40
E	43	2.28530	0.71947	-0.71601	1.07124	11,12,41,47
F	6	1.0	0.13232	0.09356	1.02609	1,5,10,41
G	44	2.57834	1.26793	0.10686	1.02228	17,41,42,43,46,47,49
H	3	0.5	-0.15272	1.58493	1.02068	1,2,5,6,7,35
I	48	3.70909	1.26732	0.90585	1.00942	16,47,50,53

Rotation symmetry is achieved only by moving atoms 35,39,48 and 53 from crystal one to crystal two. New neighbors for 35: 1,3,6,2,5; for 39: 5,6,7,9,10. The contacts and relative translation remain the same.

[111] Σ39a 32.21° (3$\bar{4}$1)



⊠ 0.871 -0.051 △ 0.768 0.058 ▽ 0.691 0.923 ⊡ 0.638 1.419 ◪ 0.615 1.277 ◪ 0.599 -0.328 △Z=-0.135



⊠ 1.171 -0.084 △ 1.062 0.084 ▽ 1.048 0.074 ⊡ 1.029 0.873

[111] $\Sigma 39a$ 32.21° $(3\bar{4}1)$ ΔZ = - 0.13546

V^{EX} = 0.45379

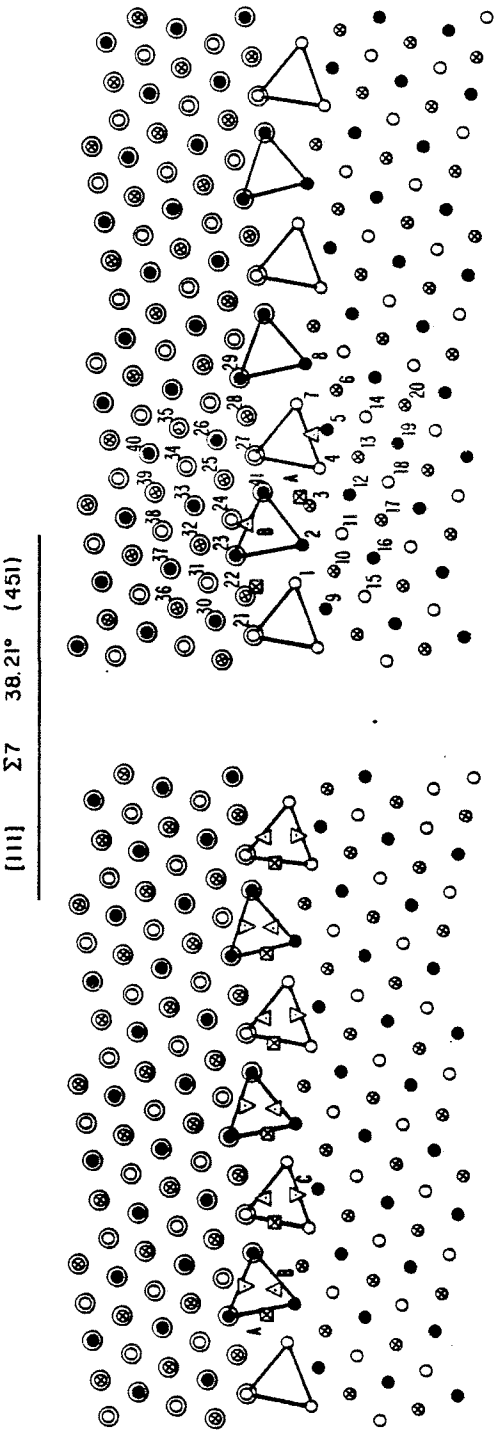
Contacts: 9-32, 7-32, 21-52

Interstitials	x	y	z	d	Touching
A	0.50832	0.79404	-0.05090	0.87066	8,9,39,40
B	-0.62737	0.01509	0.62305	0.76862	1,2,33,36
C	1.10047	1.02634	0.92341	0.69139	9,10,39,45
D	0.71584	1.34363	1.41897	0.63788	12,32,40,41
E	-0.12785	0.07381	1.27694	0.61538	2,6,7,34
F	-0.38166	0.62152	-0.32802	0.59945	1,32,34,37,39

Substitutionals		x	y	z	d	Touching
A	1	-0.10429	0.23684	-0.08370	1.17102	6,7,32,35
B	11	1.29490	0.98444	0.08373	1.06214	8,9,10,12,13,45
C	18	2.81948	1.83628	0.07370	1.04830	15,16,17,20,21,22,49
D	24	3.86130	2.96683	0.87312	1.02865	20,22,23,26,27,28,56
E	12	1.48600	1.46763	1.63299	1.02858	9,11,13,16,44
F	28	4.40339	3.80856	0.85593	1.01395	24,26,27,30,31,56
G	22	3.41997	2,64428	0.03267	1.00958	18,20,21,24,27,50
H	13	2.0	1.17874	0.80800	1.00064	11,12,15,16,17,45
I	27	3.98437	3.47313	0.00639	1.00037	22,24,28,31,57

[111] Σ39a 32.21° ($3\bar{4}1$) $\Delta Z = -0.13546$

	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.00000	-0.57735	0.81650
3	-0.50000	-0.86603	0.00000
4	-0.00000	-1.15470	1.63299
5	0.50000	-0.86603	0.00000
6	0.50000	-0.28868	1.63299
7	0.50000	0.28868	0.81650
8	1.00000	-0.00000	-0.00000
9	1.00000	0.57735	1.63299
10	1.50000	0.28868	0.81650
11	1.50000	0.86603	-0.00000
12	1.50000	1.44338	1.63299
13	2.00000	1.15470	0.81650
14	2.00000	0.57735	1.63299
15	2.50000	0.86603	-0.00000
16	2.50000	1.44338	1.63299
17	3.00000	1.15470	0.81650
18	3.00000	1.73205	-0.00000
19	3.50000	1.44338	1.63299
20	3.50000	2.02073	0.81650
21	3.00000	2.30940	1.63299
22	3.50000	2.59808	-0.00000
23	4.00000	2.30940	1.63299
24	4.00000	2.88675	0.81650
25	4.50000	2.59808	-0.00000
26	4.50000	3.17543	1.63299
27	4.00000	3.46410	-0.00000
28	4.50000	3.75278	0.81650
29	5.00000	3.46410	-0.00000
30	5.00000	4.04145	1.63299
31	4.50000	4.33013	-0.00000
32	0.05311	0.86900	1.49753
33	-0.52380	0.89140	0.68104
34	-0.83166	0.40298	1.49753
35	-1.13953	-0.08544	-0.13546
36	-1.40858	0.42539	0.68104
37	-1.10072	0.91381	-0.13546
38	-0.79285	1.40223	1.49753
39	-0.21594	1.37982	-0.13546
40	0.36098	1.35742	0.68104
41	0.09192	1.86824	1.49753
42	0.66884	1.84584	-0.13546
43	0.39979	2.35666	0.68104
44	0.97670	2.33426	1.49753
45	1.24575	1.82343	0.68104
46	1.55362	2.31185	-0.13546
47	1.28456	2.82268	0.68104
48	1.86148	2.80027	1.49753
49	2.13053	2.28944	0.68104
50	2.43839	2.77786	-0.13546
51	2.16934	3.28869	0.68104
52	2.74626	3.26628	1.49753
53	2.47720	3.77711	-0.13546
54	2.78507	4.26553	1.49753
55	3.05412	3.75470	0.68104
56	3.63103	3.73230	1.49753
57	3.36198	4.24312	-0.13546
58	3.09293	4.75395	0.68104
59	3.66984	4.73154	1.49753
60	3.40079	5.24237	-0.13546
61	3.97771	5.21996	0.68104
62	4.55462	5.19756	1.49753



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	0.28867	0.81650
3	1.00000	0.57735	1.63299
4	1.50000	0.86603	0.00000
5	2.00000	1.15470	0.81650
6	2.50000	1.44338	1.63299
7	2.00000	1.73205	0.00000
8	2.50000	2.02073	0.81650
9	-0.00000	-0.57735	0.81650
10	0.50000	-0.28867	1.63299
11	1.00000	0.00000	0.00000
12	1.50000	0.28868	0.81650
13	2.00000	0.57735	1.63299
14	2.50000	0.86603	0.00000
15	0.50000	-0.86603	0.00000
16	1.00000	-0.57735	0.81650
17	1.50000	-0.28868	1.63299
18	2.00000	-0.00000	0.00000
19	2.50000	0.28867	0.81650
20	3.00000	0.57735	1.63299
21	-0.75550	-0.05130	-0.35902
22	-0.59835	0.40226	1.27397
23	-0.24121	0.85583	0.45748
24	0.11593	1.30952	-0.35902
25	0.47308	1.76315	1.27397
26	0.83022	2.21678	0.45748
27	1.04450	1.68067	-0.35902
28	1.40164	2.13430	1.27397
29	1.75879	2.58793	0.45748
30	-1.16979	0.48473	0.45748
31	-0.81264	0.93836	-0.35902
32	-0.45549	1.39200	1.27397
33	-0.09835	1.84563	0.45748
34	0.25879	2.29926	-0.35902
35	0.61593	2.75289	1.27397
36	-1.38407	1.02084	1.27397
37	-1.02693	1.47447	0.45748
38	-0.66979	1.92810	-0.35902
39	-0.31264	2.38173	1.27397
40	0.04451	2.83537	0.45748
41	0.68736	1.22703	0.45748

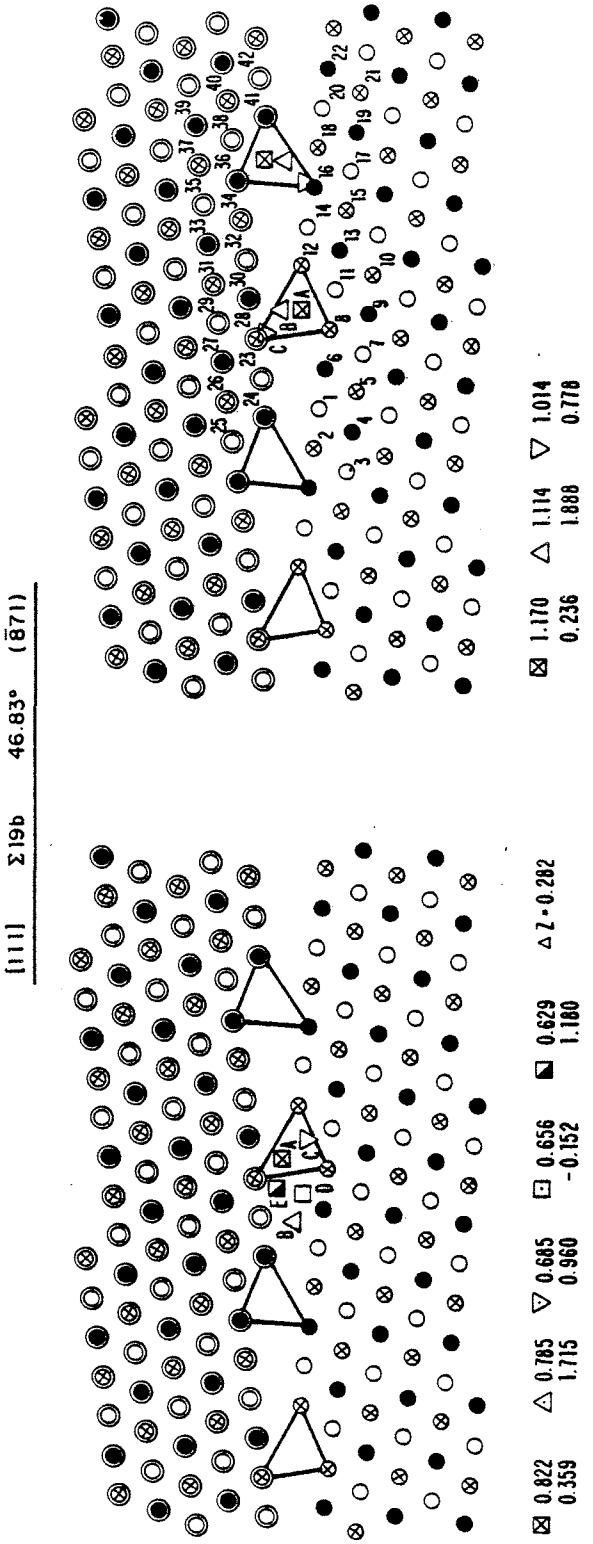
[111] $\Sigma 7$ 38.21° $(4\bar{5}1)$ $\Delta z = -0.35902$

$$V^{EX} = 0.41358$$

Contacts: 1-23, 2-23, 4-27, 4-41.

Interstitials	x	y	z	d	Touching
A	0.13376	0.50413	1.74505	0.75304	1,3,22,24
B	0.50000	0.64213	-0.08286	0.63608	1,11,24,41
C	1.71614	1.31858	1.80947	0.62623	4,6,7,13,27
D	0.98282	0.58727	0.39422	0.41505	2,4,11,41

Substitutionals		x	y	z	d	Touching
A	3	1.00000	0.80493	1.55253	1.05744	2,4,12,13,27
B	24	0.19953	1.10037	-0.43865	1.05628	3,23,25,27,31,32,41



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.28868	1.63299
3	-0.50000	-0.86603	0.00000
4	0.00000	-0.57735	0.81650
5	0.50000	-0.28868	1.63299
6	0.50000	0.28868	0.81650
7	1.00000	0.00000	0.00000
8	1.00000	0.57735	1.63299
9	1.50000	0.28868	0.81650
10	2.00000	0.57735	1.63299
11	1.50000	0.86603	0.00000
12	1.50000	1.44338	1.63299
13	2.00000	1.15470	0.81650
14	2.00000	1.73205	-0.00000
15	2.50000	1.44338	1.63299
16	2.50000	2.02073	0.81650
17	3.00000	1.73205	-0.00000
18	3.00000	2.30940	1.63299
19	3.50000	2.02073	0.81650
20	3.50000	2.59808	-0.00000
21	4.00000	2.30940	1.63299
22	4.00000	2.88675	0.81650
23	-0.13373	0.94995	0.28232
24	-0.55478	0.55492	1.09882
25	-1.10741	0.72205	0.28232
26	-0.68636	1.11708	-0.53417
27	-0.26531	1.51211	1.09882
28	0.28732	1.34498	-0.53417
29	0.15575	1.90714	0.28232
30	0.70838	1.74001	1.09882
31	0.57680	2.30217	-0.53417
32	1.12943	2.13504	0.28232
33	0.99785	2.69720	1.09882
34	1.55048	2.53007	-0.53417
35	1.41890	3.09222	0.28232
36	1.97154	2.92510	1.09882
37	1.83996	3.48725	-0.53417
38	2.39259	3.32013	0.28232
39	2.26101	3.88228	1.09882
40	2.81364	3.71515	-0.53417
41	2.94522	3.15300	1.09882
42	3.36627	3.54803	0.28232

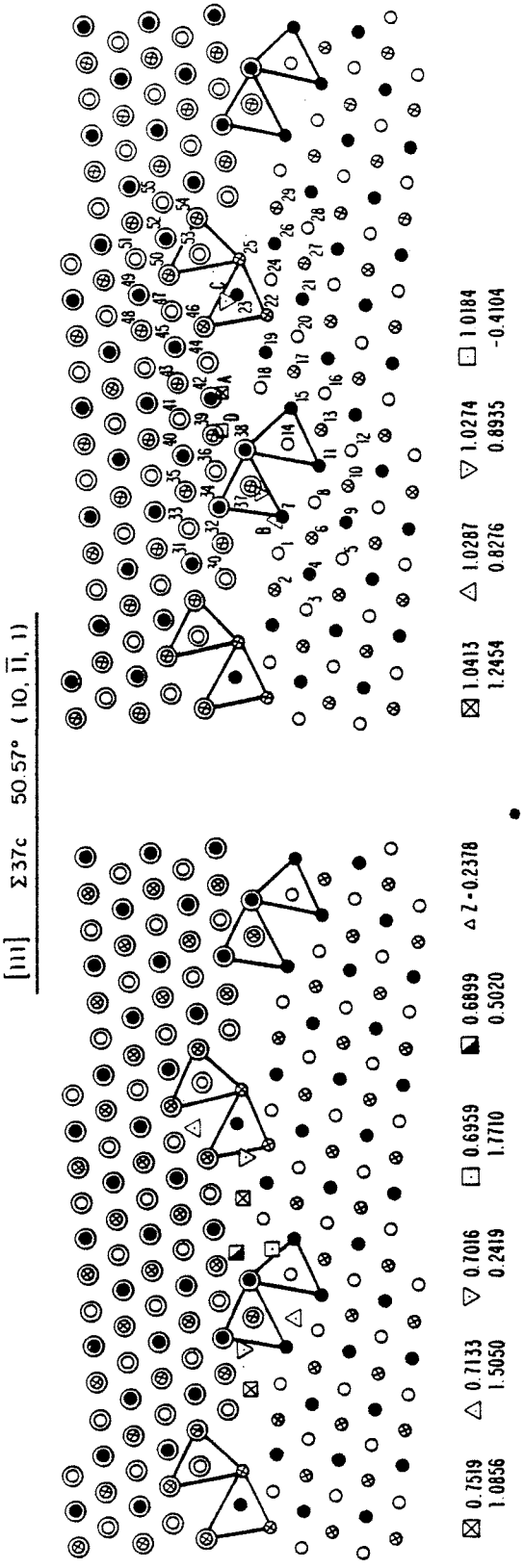
[111] $\Sigma 19b$ 46.83° $(7\bar{8}1)$ $\Delta Z = 0.28232$

$V^{EX} = 0.49963$

Contacts: 1-23, 14-32, 2-24, 12-30.

Interstitials	x	y	z	d	Touching
A	0.73624	1.20922	0.35894	0.82202	11,23,29,30
B	0.08823	0.49864	1.71485	0.78451	1,5,24,28
C	1.17607	1.05305	0.96026	0.68506	8,9,12,13,30
D	0.5	0.64198	-0.15225	0.65567	1,7,23,28
E	0.36684	1.00525	1.17959	0.62855	6,27,28,30
F	0.95687	1.66486	2.13999	0.55061	12,28,31,32
G	1.44601	1.47455	0.43029	0.49448	11,13,14,32
H	0.97641	1.16832	-0.39862	0.44835	8,11,12,28
I	1.14713	2.05941	-0.88750	0.42695	12,30,31,34

Substitutionals		x	y	z	d	Touching
A	11	0.99638	1.05903	0.23565	1.17000	6,7,28,32
B	30	0.81181	1.29813	0.84416	1.11374	6,12,29,32
C	28	0.39254	1.31316	-0.49531	1.01355	8,23,29,30,31
D	6	0.42210	0.33365	0.84830	1.00908	1,4,5,8,23
E	8	0.93043	0.61752	1.66140	1.00724	5,6,7,11,12,28



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.28868	1.63299
3	-0.50000	-0.86603	0.00000
4	0.00000	-0.57735	0.81650
5	0.50000	-0.86603	0.00000
6	0.50000	-0.28868	1.63299
7	0.50000	0.28868	0.81650
8	1.00000	0.00000	-0.00000
9	1.00000	-0.57735	0.81650
10	1.50000	-0.28868	1.63299
11	1.50000	0.28868	0.81650
12	2.00000	-0.00000	-0.00000
13	2.00000	0.57735	1.63299
14	1.50000	0.86603	-0.00000
15	2.00000	1.15470	0.81650
16	2.50000	0.86603	-0.00000
17	2.50000	1.44338	1.63299
18	2.00000	1.73205	-0.00000
19	2.50000	2.02073	0.81650
20	3.00000	1.73205	-0.00000
21	3.50000	2.02073	0.81650
22	3.00000	2.30940	1.63299
23	3.00000	2.88675	0.81650
24	3.50000	2.59808	-0.00000
25	3.50000	3.17543	1.63299
26	4.00000	2.88675	0.81650
27	4.00000	2.30940	1.63299
28	4.50000	2.59808	-0.00000
29	4.50000	3.17543	1.63299
30	-0.81462	0.45412	0.36079
31	-0.90921	1.02367	1.17729
32	-0.36867	0.82082	-0.45571
33	-0.46327	1.39036	0.36079
34	0.07727	1.18751	1.17729
35	-0.01732	1.75706	-0.45571
36	0.52322	1.55421	0.36079
37	0.61781	0.98466	-0.45571
38	1.06376	1.35135	1.17729
39	0.96916	1.92090	-0.45571
40	0.42862	2.12375	1.17729
41	0.87457	2.49045	0.36079
42	1.41511	2.28760	1.17729
43	1.32052	2.85714	-0.45571
44	1.86106	2.65429	0.36079
45	1.76646	3.22384	1.17729
46	2.30700	3.02099	-0.45571
47	2.21241	3.59054	0.36079
48	1.67187	3.79339	-0.45571
49	2.11781	4.16008	1.17729
50	2.65835	3.95723	-0.45571
51	2.56376	4.52678	0.36079
52	3.10430	4.32393	1.17729
53	3.19889	3.75438	0.36079
54	3.64484	4.12107	-0.45571
55	3.55025	4.69062	0.36079

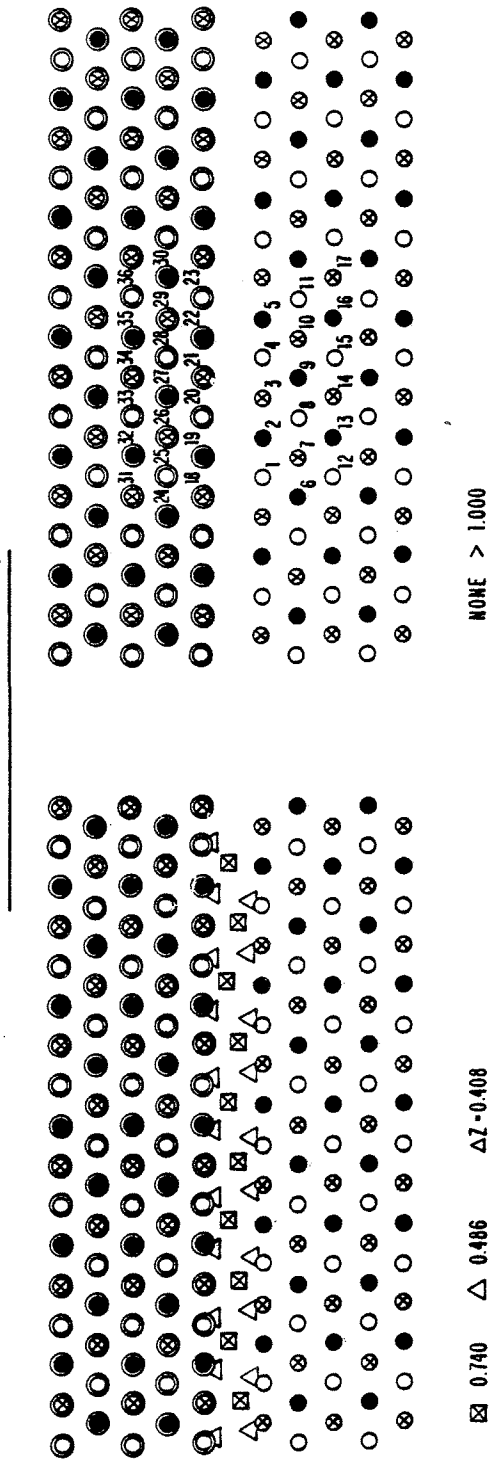
[111] $\Sigma 37c$ 50.57° $(10,\bar{1}\bar{1},1)$ $\Delta z = 0.36079$

$V^{EX} = 0.46030$

Contacts: 1-30, 18-44, 14-37

Interstitials	x	y	z	d	Touching
A	-0.32931	0.37353	1.08560	0.75191	2,7,30,31
B	1.00003	0.39487	1.50496	0.71332	6,7,10,11,37
C	0.14107	0.80340	0.24194	0.70163	1,7,33,36
D	1.66909	1.34576	1.77105	0.69588	13,14,17,18,38
E	1.32271	1.78822	0.50202	0.68985	18,36,38,41,42
F	2.35836	2.67985	1.26265	0.61686	19,23,45,46
G	0.92563	0.89764	0.54364	0.58297	7,14,36,38
H	1.31420	0.88453	1.71680	0.51222	13,14,37,38
I	1.94482	1.76391	1.24727	0.49632	15,17,19,42
J	1.43361	2.17621	0.03238	0.44101	18,39,41,44

Substitutionals		x	y	z	d	Touching
A	42	1.59549	2.21990	1.24540	1.04133	19,38,39,43,44,45
B	7	0.48646	0.32776	0.82755	1.02871	1,6,11,34
C	23	2.82078	2.97926	0.89354	1.02742	19,22,47,53
D	39	1.08926	1.87583	-0.41035	1.01842	18,36,37,38,41,42,43
E	38	1.07751	1.33995	1.17251	1.01200	15,36,37,42
F	22	2.95333	2.33635	1.65205	1.00326	17,19,20,23,24,25,46
G	15	1.98104	1.16565	0.82424	1.00054	11,13,14,17,18,19,38
H	19	2.48942	2.02683	0.82081	1.00016	15,17,18,22,23,44



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	0.28867	0.81650
3	1.00000	0.57735	1.63299
4	1.50000	0.86603	0.00000
5	2.00000	1.15470	0.81650
6	-0.00000	-0.57735	0.81650
7	0.50000	-0.28867	1.63299
8	1.00000	0.00000	0.00000
9	1.50000	0.28868	0.81650
10	2.00000	0.57735	1.63299
11	2.50000	0.86603	0.00000
12	0.50000	-0.86603	0.00000
13	1.00000	-0.57735	0.81650
14	1.50000	-0.28868	1.63299
15	2.00000	-0.00000	0.00000
16	2.50000	0.28867	0.81650
17	3.00000	0.57735	1.63299
18	-0.68302	0.60566	2.04124
19	-0.18301	0.89434	1.22475
20	0.31699	1.18302	0.40825
21	0.81699	1.47169	2.04124
22	1.31699	1.76037	1.22475
23	1.81699	2.04904	0.40825
24	-1.18301	0.89434	1.22475
25	-0.68301	1.18302	0.40825
26	-0.18302	1.47169	2.04124
27	0.31698	1.76037	1.22475
28	0.81698	2.04904	0.40825
29	1.31698	2.33772	2.04124
30	1.81698	2.62639	1.22475
31	-1.18302	1.47169	2.04124
32	-0.68301	1.76037	1.22475
33	-0.18301	2.04904	0.40825
34	0.31699	2.33772	2.04124
35	0.81699	2.62639	1.22475
36	1.31699	2.91507	0.40825

[111] $\Sigma 3$ 60.00° $(1\bar{1}0)$ $\Delta z = 0.40825$

$v^{EX} = 0.4108$

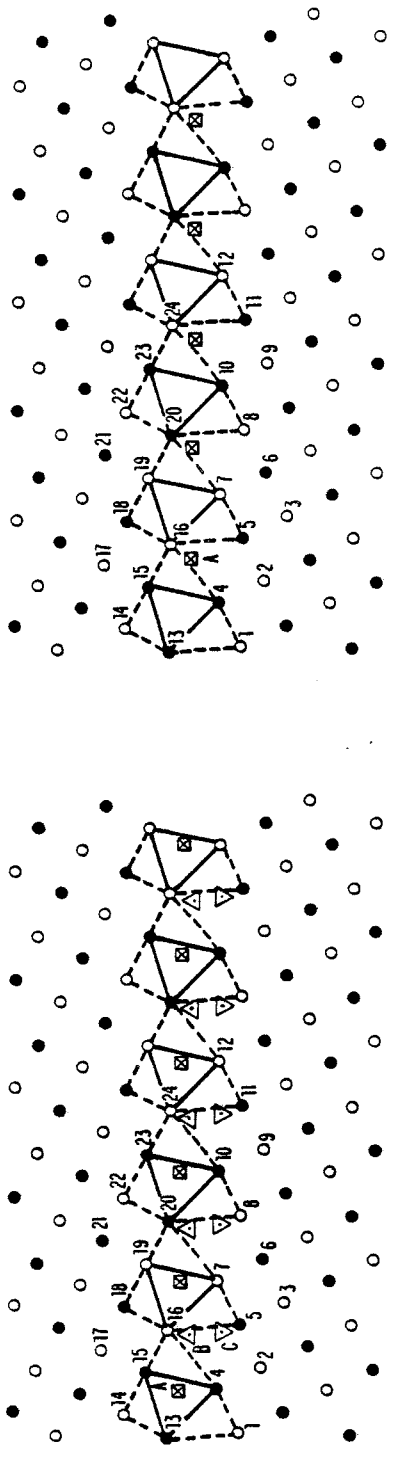
Contacts: 2-19, 3-21, 2-20, 4-21'

Interstitials	x	y	z	d	Touching
A	0.29019	0.74489	-0.34261	0.73950	1,3,20,26
B	0.83861	0.67053	0.27648	0.48606	2,4,8,20

Substitutionals	x	y	z	d	Touching
none > 1.0000					

5.4 LESS DENSE BOUNDARIES

[100] and [110] boundaries, each listed in order of increasing Σ



	X	Y	Z
1	0.0	0.0	0.0
2	1.0	0.0	0.0
3	2.0	0.0	0.0
4	0.5	0.5	0.70711
5	1.5	0.5	0.70711
6	2.5	0.5	0.70711
7	2.0	1.0	0.0
8	3.0	1.0	0.0
9	4.0	1.0	0.0
10	3.5	1.5	0.70711
11	4.5	1.5	0.70711
12	5.0	2.0	0.0
13	-0.41962	0.89282	0.70711
14	-0.31962	1.59282	0.0
15	0.38038	1.49282	0.70711
16	1.08038	1.39282	0.0
17	0.48038	2.19282	0.0
18	1.18038	2.09282	0.70711
19	1.88038	1.99282	0.0
20	2.58038	1.89282	0.70711
21	1.98038	2.69282	0.70711
22	2.68038	2.59282	0.0
23	3.38038	2.49282	0.70711
24	4.08038	2.39282	0.0

[100] $\Sigma 5$ 53.13° (021) $\Delta z = 0$

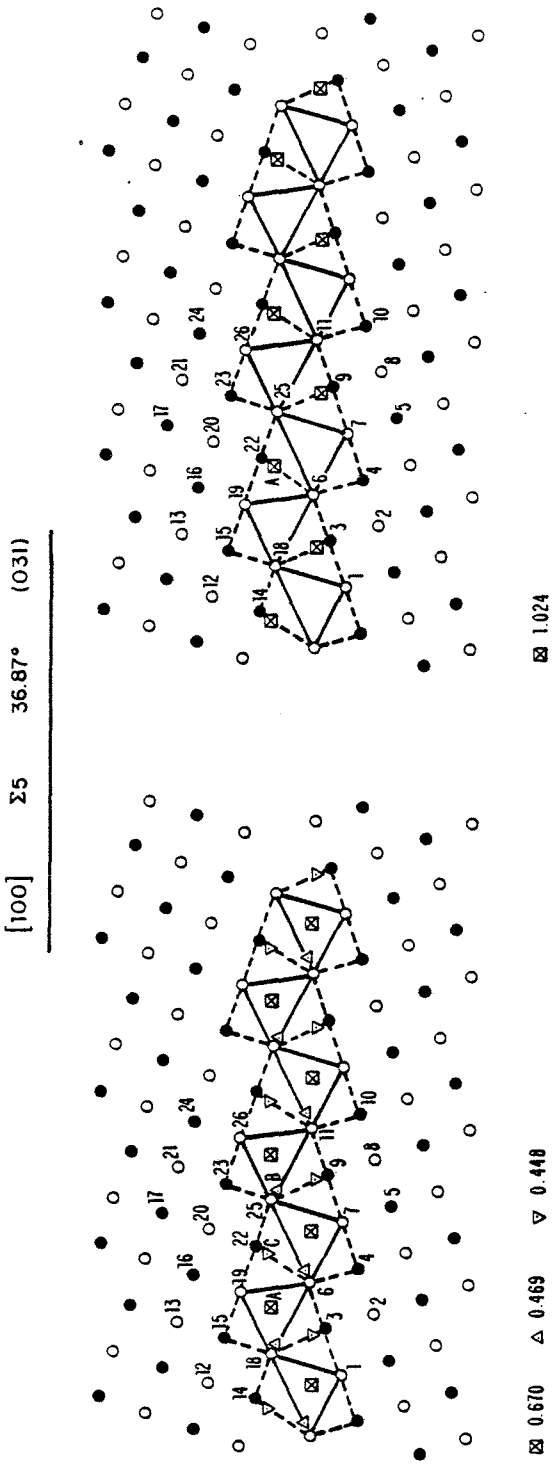
$v^{EX} = 0.3898$

Not the densest

Contacts: 4-13, 4-15

Interstitials	x	y	z	d	Touching
A	0.30717	0.98038	0.0	0.75265	4,4',14,15,15',16
B	1.03980	1.10874	0.70711	0.52624	5,15,16,16'
C	1.31972	0.68028	0.0	0.50333	2,5,5',7,16

Substitutionals		x	y	z	d	Touching
A	16	.97954	1.06139	0.0	1.04462	4,4',7,15,15'



	X	Y	Z
1	0.00000	0.00000	0.70711
2	1.0	0.0	0.70711
3	0.5	0.5	0.0
4	1.5	0.5	0.0
5	2.5	0.5	0.0
6	1.0	1.0	0.70711
7	2.0	1.0	0.70711
8	3.0	1.0	0.70711
9	2.5	1.5	0.0
10	3.5	1.5	0.0
11	3.0	2.0	0.70711
12	-1.0359	1.5718	0.70711
13	-0.4359	2.3718	0.70711
14	-0.9359	0.8718	0.0
15	-0.3359	1.6718	0.0
16	0.2641	2.4718	0.0
17	0.8641	3.2718	0.0
18	-0.2359	0.9718	0.70711
19	0.3641	1.7718	0.70711
20	0.9641	2.5718	0.70711
21	1.5641	3.3718	0.70711
22	1.0641	1.8718	0.0
23	1.6641	2.6718	0.0
24	2.2641	3.4718	0.0
25	1.7641	1.9718	0.70711
26	2.3641	2.7718	0.70711

[100] $\Sigma 5$ 36.87° (031) $\Delta Z = 0$

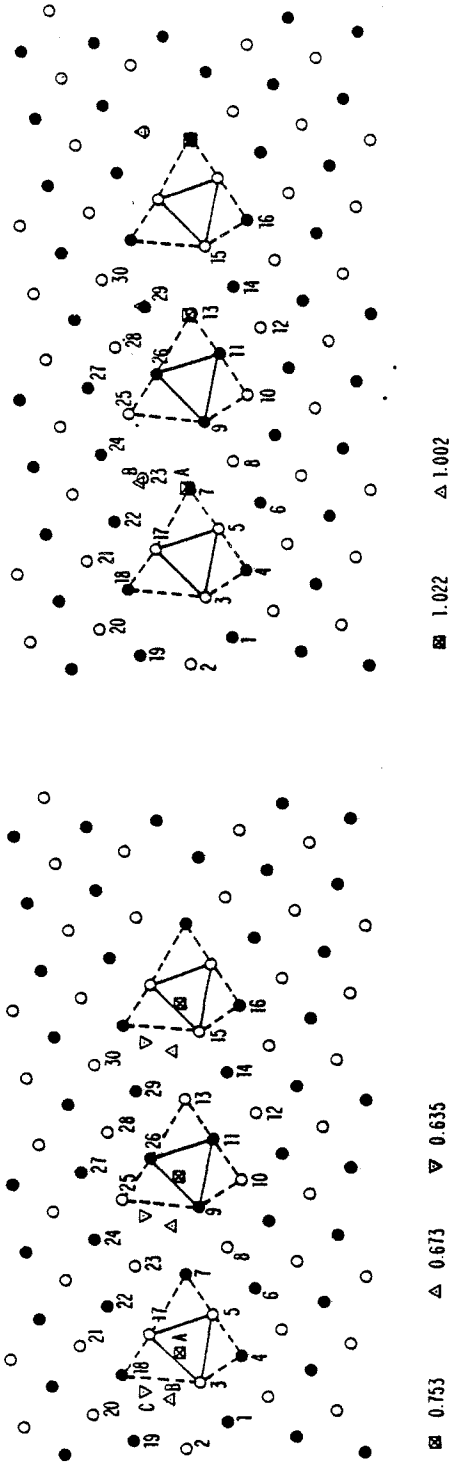
$V^{EX} = 0.3411$

Not the densest

Contacts: 1-18, 6-19

Interstitials	x	y	z	d	Touching
A	0.42694	1.33193	0.0	0.67025	3,15,19,19',22
A'	1.68581	1.31420	0.0		4,7,7',9,22
B	1.96167	2.00003	0.0	0.46946	9,23,25,25'
B'	1.14112	1.14112	0.0		4,6,6',22
C	1.08597	1.71870	0.70711	0.44764	6,19,22,22',25
C'	2.39064	1.60936	0.70711		7,9,9',11,25

Substitutionals		x	y	z	d	Touching
A	22	1.08597	1.71870	0.0	1.02378	6,6',19,19',25,25'
A'	9	2.39064	1.60936	0.0		7,7',11,11',25,25'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	0.50000	0.70711
3	0.50000	0.50000	0.70711
4	1.00000	0.00000	0.00000
5	1.50000	0.50000	0.70711
6	2.00000	0.00000	0.00000
7	2.00000	1.00000	0.00000
8	2.50000	0.50000	0.70711
9	3.00000	1.00000	0.00000
10	3.50000	0.50000	0.70711
11	4.00000	1.00000	0.00000
12	4.50000	0.50000	0.70711
13	4.50000	1.50000	0.70711
14	5.00000	1.00000	0.00000
15	5.50000	1.50000	0.70711
16	6.00000	1.00000	0.00000
17	1.00000	1.36603	0.70711
18	0.34615	1.63526	0.00000
19	-0.57692	1.25064	0.00000
20	-0.30769	1.90449	0.70711
21	0.61538	2.28910	0.70711
22	1.26923	2.01987	0.00000
23	1.92308	1.75064	0.70711
24	2.19231	2.40449	0.00000
25	2.84615	2.13526	0.70711
26	3.50000	1.86603	0.00000
27	3.11538	2.78910	0.00000
28	3.76923	2.51987	0.70711
29	4.42308	2.25064	0.00000
30	4.69231	2.90449	0.70711

[100] $\Sigma 13a$ 67.38° (023) $\Delta Z = 0$

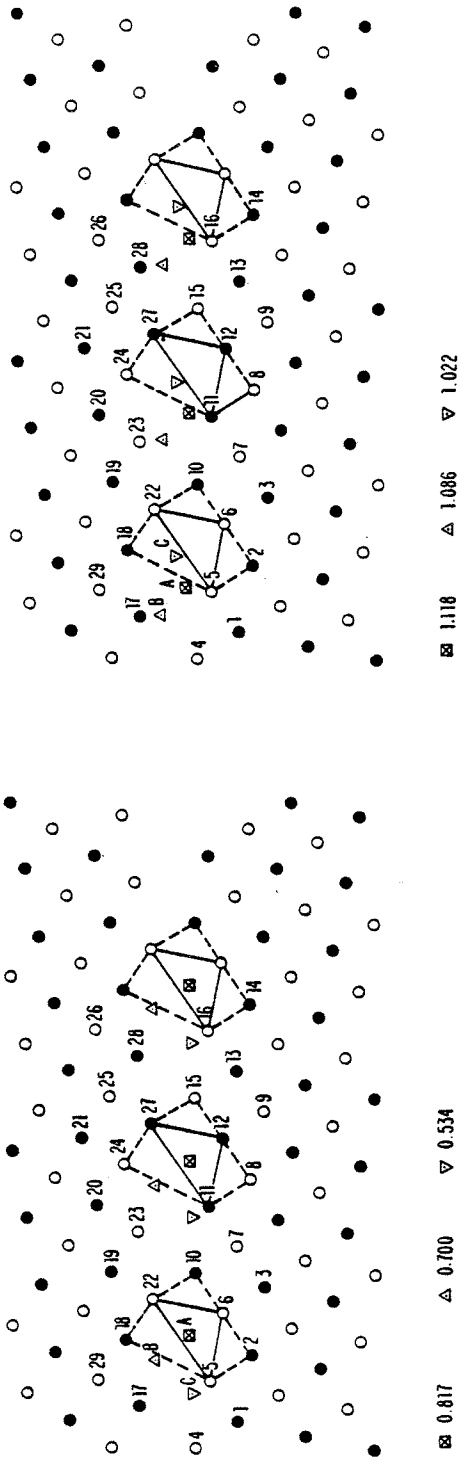
$V^{EX} = 0.40287$

Second densest

Contacts: 3-17, 5-17

Interstitials	x	y	z	d	Touching
A	0.86585	0.86673	0.0	0.75309	3,3',4,17,17'
B	0.14247	0.82411	0.02364	0.67333	1,3,18,19
C	0.19010	1.25627	0.70711	0.63461	3,17,18,18',20

Substitutionals		x	y	z	d	Touching
A	7	1.98958	1.03126	0.0	1.02181	5,5',9,23,23'
B	23	1.94154	1.70632	0.70711	1.00230	7,7',17,25



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.0	0.0	0.0
3	2.0	0.0	0.0
4	-0.5	0.5	0.70711
5	0.5	0.5	0.70711
6	1.5	0.5	0.70711
7	2.5	0.5	0.70711
8	3.5	0.5	0.70711
9	4.5	0.5	0.70711
10	2.0	1.0	0.0
11	3.0	1.0	0.0
12	4.0	1.0	0.0
13	5.0	1.0	0.0
14	6.0	1.0	0.0
15	4.5	1.5	0.70711
16	5.5	1.5	0.70711
17	-0.0769	1.3846	0.0
18	0.8462	1.77692	0.0
19	1.7693	2.1538	0.0
20	2.6924	2.5384	0.0
21	3.6154	2.9230	0.0
22	1.5	1.5	0.70711
23	2.4231	1.8846	0.70711
24	3.3462	2.2692	0.70711
25	4.2692	2.6538	0.70711
26	5.1923	3.0385	0.70711
27	4.0	2.0	0.0
28	4.9231	2.3846	0.0
29	0.1924	2.0384	0.70711

[100] Σ13a 67.38° (023) $\Delta Z = 0.0$

$V^{EX} = 0.4402$

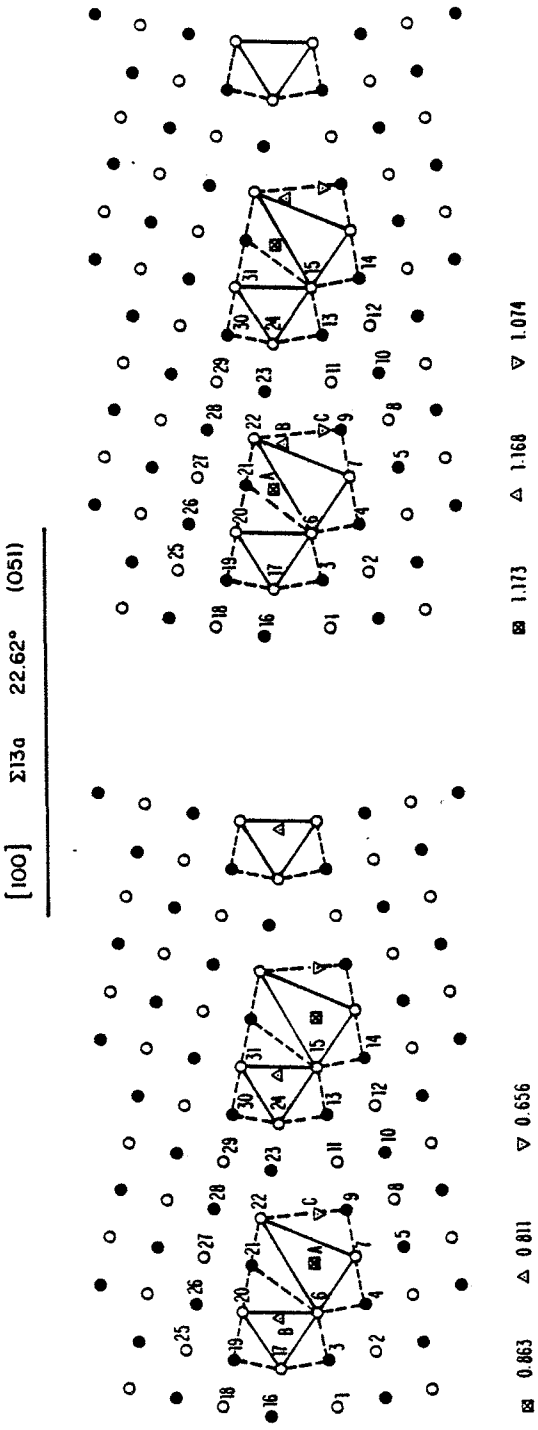
Third densest

Contacts: 6-22, 10-22, 10-22'

Interstitials	x	y	z	d	Touching
A	1.09653	0.90347	0.0	0.81723	2,6,6',10,18
B	0.66671	1.33329	0.70225	0.69963	5,18,18',22,29
C	0.28948	0.710513	0.0	0.53444	1,5,5',17
(D)	2.17647	1.17647	0.70711	0.49971	7,10,10',22,23

Substitutionals		x	y	z	d	Touching
A	5	0.5	0.84780	0.70711	1.11751	4,6,17,17'
B	17	0.03704	1.11130	0.0	1.08596	5,5',18,unnumbered
B'	23					11,11',22,24
C	18	0.89475	1.10525	0.0	1.02203	5,5',17,22,22'

Lattices exactly on the coincidence lattice; CSL sites: 22,27



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	0.50000	0.50000	0.70711
4	1.50000	0.50000	0.70711
5	2.50000	0.50000	0.70711
6	1.00000	1.00000	0.00000
7	2.00000	1.00000	0.00000
8	3.00000	1.00000	0.00000
9	2.50000	1.50000	0.70711
10	3.50000	1.50000	0.70711
11	3.00000	2.00000	0.00000
12	4.00000	2.00000	0.00000
13	3.50000	2.50000	0.70711
14	4.50000	2.50000	0.70711
15	4.00000	3.00000	0.00000
16	-0.65385	0.73077	0.70711
17	0.00000	1.00000	0.00000
18	-0.92308	1.38462	0.00000
19	-0.26923	1.65385	0.70711
20	0.38462	1.92308	0.00000
21	1.03847	2.19231	0.70711
22	1.69232	2.46154	0.00000
23	2.34617	2.73077	0.70711
24	3.00000	3.00000	0.00000
25	-0.53846	2.30770	0.00000
26	0.11539	2.57693	0.70711
27	0.76924	2.84616	0.00000
28	1.42309	3.11539	0.70711
29	2.07694	3.38462	0.00000
30	2.73079	3.65385	0.70711
31	3.38464	3.92308	0.00000

[100] $\Sigma 13$ 22.62° (051) $\Delta Z = 0.0$

$V^{EX} = 0.4760$

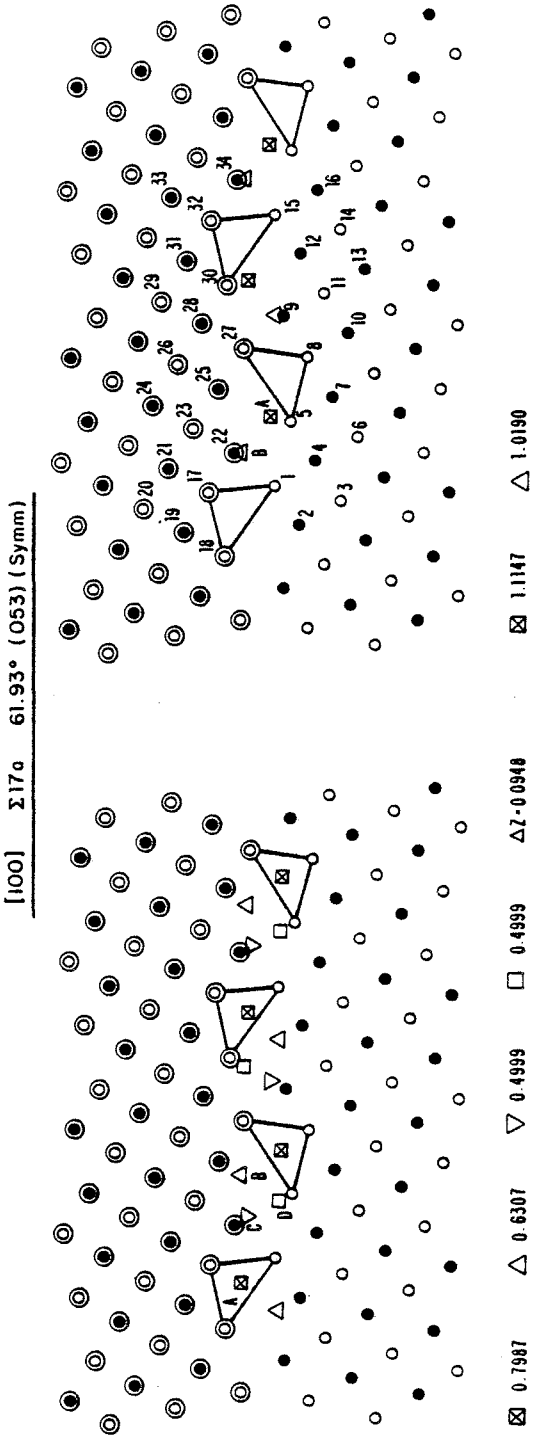
Not the densest

Contacts: 1-17, 3-17, 6-17

Interstitials	x	y	z	d	Touching
A	1.57140	1.42860	0.70711	0.86267	4,7,7',9,21
B	0.60000	1.40000	0.70711	0.81110	3,6,6',19,20,20',21
C	2.19560	1.80440	0.0	0.65567	7,9,9',11,22
D	1.19998	1.80002	0.0	0.64928	6,20,21,21',22
E	2.44115	2.50002	0.0	0.49978	11,22,23,23',24
F	2.83333	2.16666	0.70711	0.49071	9,11,11',13,23

Substitutionals		x	y	z	d	Touching
A	21	1.2	1.8	0.70711	1.17255	6,6',20,20',22,22'
B	22	1.85186	2.07407	0.0	1.16848	7,21,21',23,23'
C	9	2.30555	1.69444	0.70711	1.07423	7,7',11,11',23
D	23	2.43183	2.52273	0.70710	1.04999	9,22,22',24,24'
E	6	1.0	1.125	0.08839	1.02330	3,4,7,17,20

Lattices exactly on the coincidence lattice; CSL sites 17,5,24



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.50000	0.70711
3	0.00000	-1.00000	0.00000
4	0.50000	-0.50000	0.70711
5	1.00000	0.00000	0.00000
6	1.00000	-1.00000	0.00000
7	1.50000	-0.50000	0.70711
8	2.00000	0.00000	0.00000
9	2.50000	0.50000	0.70711
10	2.50000	-0.50000	0.70711
11	3.00000	0.00000	0.00000
12	3.50000	0.50000	0.70711
13	3.50000	-0.50000	0.70711
14	4.00000	0.00000	0.00000
15	4.00000	1.00000	0.00000
16	4.50000	0.50000	0.70711
17	-0.35729	0.92917	0.09476
18	-1.23965	0.45858	0.09476
19	-1.03376	1.13506	-0.61235
20	-0.82788	1.81153	0.09476
21	-0.15141	1.60564	-0.61235
22	0.31918	0.72329	-0.61235
23	0.52506	1.39976	0.09476
24	0.73094	2.07623	-0.61235
25	1.20153	1.19388	-0.61235
26	1.40741	1.87035	0.09476
27	1.87800	0.98800	0.09476
28	2.08388	1.66447	-0.61235
29	2.28977	2.34094	0.09476
30	2.76035	1.45858	0.09476
31	2.96624	2.13505	-0.61235
32	3.64271	1.92917	0.09476
33	3.84859	2.60564	-0.61235
34	4.31918	1.72329	-0.61235

[100] Σ17a 61.93° (053) $\Delta z = 0.09476$

Symmetrical

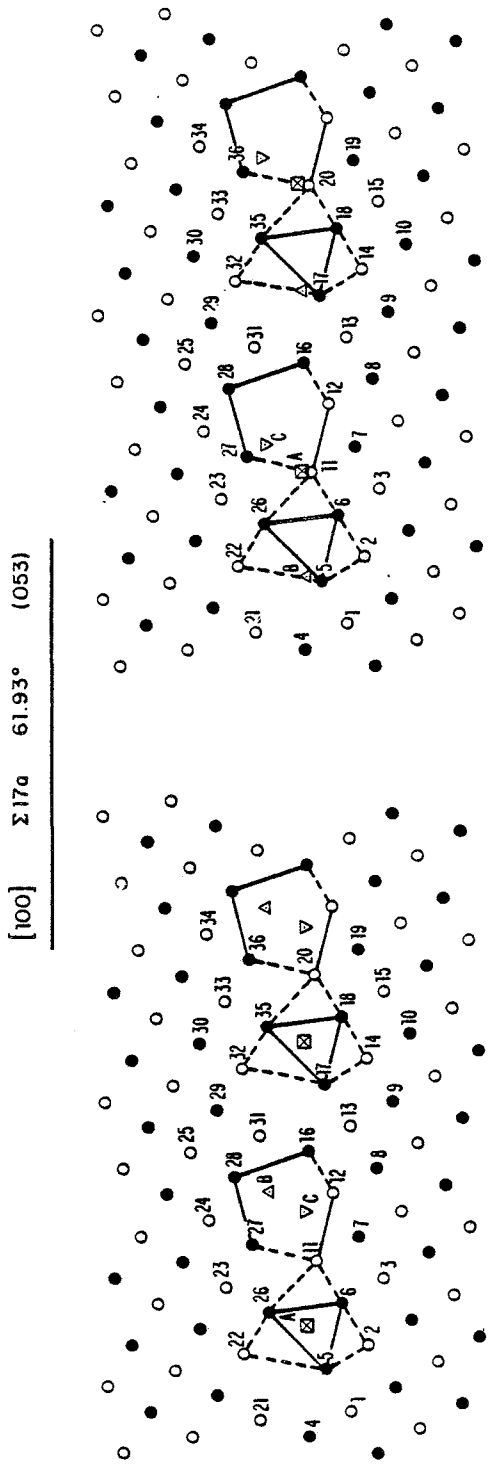
$V^{EX} = 0.42850$

Second densest

Contacts: 1-17, 8-27, 1-22, 9-27

Interstitials	x	y	z	d	Touching
A	-0.52361	0.39440	0.79847	0.79872	1,2,17,19
B	1.08334	0.80552	0.09476	0.63069	5,23,25,25',27
C	0.5	0.55086	0.09476	0.49990	1,5,22,22'
D	0.82347	0.17661	0.70711	0.49990	4,5,5',22
(E)	1.96496	0.96154	0.80187	0.42584	9,27,27',28

Substitutionals		x	y	z	d	Touching
A	5	1.0	0.33022	0.09476	1.11473	1,8,22,22'
B	9	2.50350	0.63052	0.80187	1.01895	11,12,27,27'



	X	Y	Z
1	0.00000	0.00000	0.70711
2	1.0	0.0	0.70711
3	2.0	0.0	0.70711
4	-0.5	0.5	0.0
5	0.5	0.5	0.0
6	1.5	0.5	0.0
7	2.5	0.5	0.0
8	3.5	0.5	0.0
9	4.5	0.5	0.0
10	5.5	0.5	0.0
11	2.0	1.0	0.70711
12	3.0	1.0	0.70711
13	4.0	1.0	0.70711
14	5.0	1.0	0.70711
15	6.0	1.0	0.70711
16	3.5	1.5	0.0
17	4.5	1.5	0.0
18	5.5	1.5	0.0
19	6.5	1.5	0.0
20	6.0	2.0	0.70711
21	-0.3521	1.1914	0.70711
22	0.5303	1.6620	0.70711
23	1.4127	2.1326	0.70711
24	2.2950	2.6032	0.70711
25	3.1774	3.0737	0.70711
26	1.2068	1.4561	0.0
27	2.0892	1.9267	0.0
28	2.9715	2.3973	0.0
29	3.8539	2.8679	0.0
30	4.7362	3.3385	0.0
31	3.6480	2.1914	0.70711
32	4.5303	2.6620	0.70711
33	5.4127	3.1326	0.70711
34	6.2950	3.6032	0.70711
35	5.2068	2.4561	0.0
36	6.0891	2.9267	0.0

[100] $\Sigma 17_a$ 61.93° (053) $\Delta Z = 0$

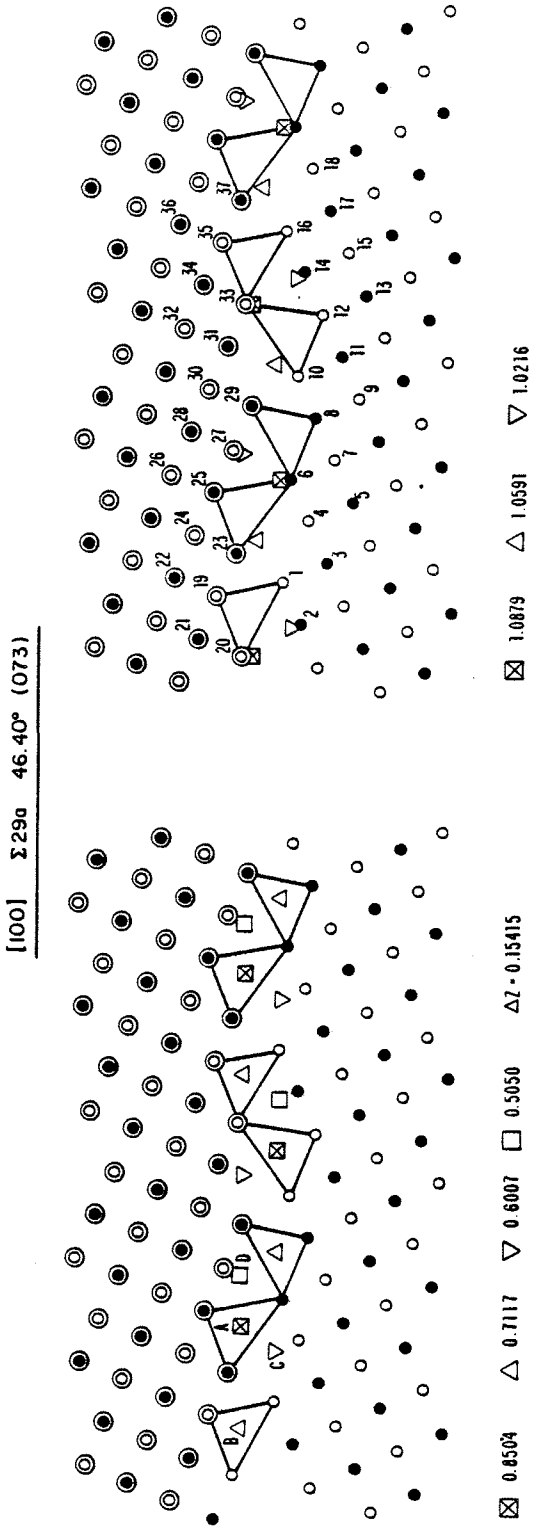
$v^{EX} = 0.4404$

Third densest

Contacts: 6-26, 16-31

Interstitials	x	y	z	d	Touching
A	1.04016	0.90872	0.70711	0.81922	6,22,26,26'
B	2.81220	1.87403	0.70711	0.78795	12,24,28,28',31
C	2.67664	1.32335	0.0	0.68418	7,12,12',16,27
(D)	4.41975	2.29863	0.0	0.60530	17,29,32,32',35
(E)	4.27195	1.72805	0.70711	0.55436	13,17,17',31
(F)	1.90640	1.20688	0.0	0.48534	11,11',26,27
(G)	2.03066	1.73447	0.70711	0.47021	11,23,27,27'

Substitutionals		x	y	z	d	Touching
A	11	1.95032	1.14904	0.70711	1.12042	6,6',12,27,27'
B	5	0.5	0.71634	0.15298	1.06902	1,2,4,6,26
C	27	2.20039	1.71814	0.0	1.05512	11,11',26,28
(D)	12	2.78557	1.6835	0.67717	1.00264	16,27,28,31 close to 11,24,27',28'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.50000	0.70711
3	0.50000	-0.50000	0.70711
4	1.00000	-0.00000	0.00000
5	1.50000	-0.50000	0.70711
6	1.50000	0.50000	0.70711
7	2.00000	0.00000	0.00000
8	2.50000	0.50000	0.70711
9	3.00000	0.00000	0.00000
10	3.00000	1.00000	0.00000
11	3.50000	0.50000	0.70711
12	4.00000	1.00000	0.00000
13	4.50000	0.50000	0.70711
14	4.50000	1.50000	0.70711
15	5.00000	1.00000	0.00000
16	5.00000	2.00000	0.00000
17	5.50000	1.50000	0.70711
18	6.00000	2.00000	0.00000
19	-0.53283	0.83207	0.15415
20	-1.25696	0.14241	0.15415
21	-1.23972	0.84931	-0.55296
22	-0.51558	1.53896	-0.55296
23	0.17407	0.81482	-0.55296
24	0.19131	1.52172	0.15415
25	0.89821	1.50448	-0.55296
26	0.91545	2.21138	0.15415
27	1.60511	1.48724	0.15415
28	1.62235	2.19414	-0.55296
29	2.31200	1.47000	-0.55296
30	2.32924	2.17690	0.15415
31	3.03614	2.15965	-0.55296
32	3.05338	2.86655	0.15415
33	3.74304	2.14241	0.15415
34	3.76028	2.84931	-0.55296
35	4.46717	2.83207	0.15415
36	4.48442	3.53897	-0.55296
37	5.17407	2.81483	-0.55296

[100] Σ29a 46.40° (073) Δz = 0.15415

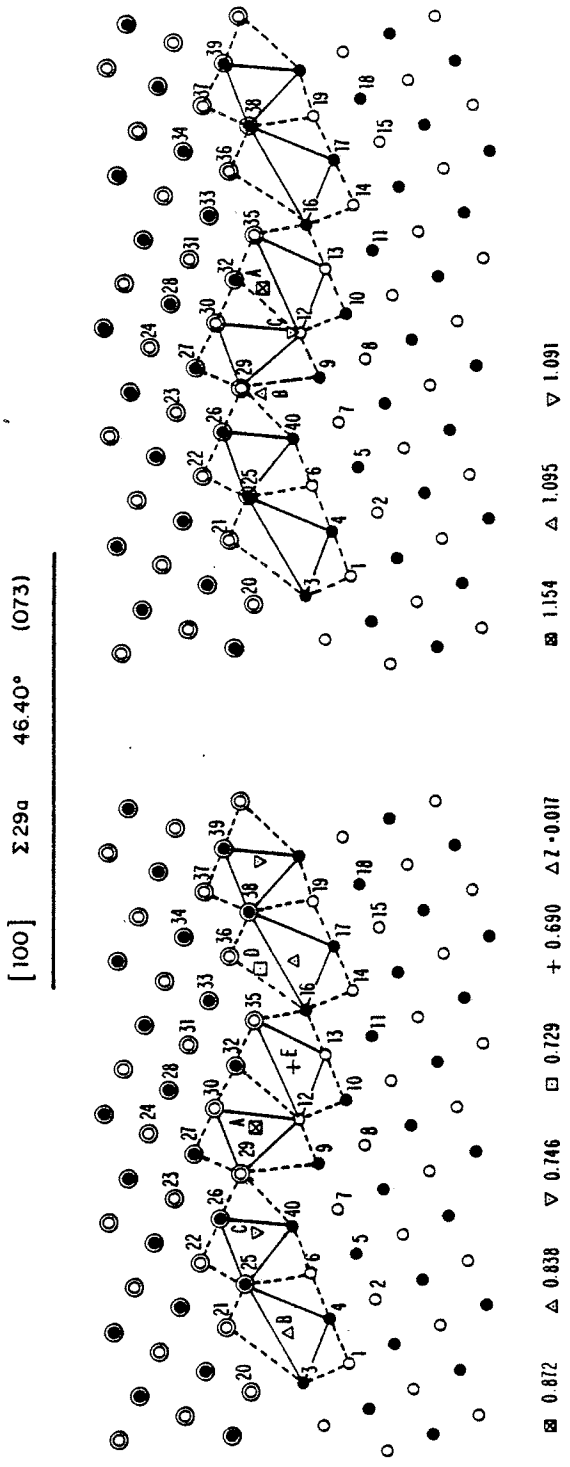
v^{EX} = 0.46398

Second densest

Contacts: 1-19,1-23,8-29,10-29

Interstitials	x	y	z	d	Touching
A	0.88090	0.90491	0.15146	0.85039	4,6,24,25
B	-0.55086	0.34143	-0.55902	0.71174	1,2,19,21
C	0.73492	0.26508	0.70711	0.60066	3,4,4',6,23
D	1.59883	1.22989	-0.55296	0.50501	6,25,27,27',29
E	0.11022	0.11022	0.70711	0.44817	1,1',3,23
F	0.17082	0.68175	0.15415	0.43905	1,19,23,23'

Substitutionals		x	y	z	d	Touching
A	6	1.46221	0.61336	0.70711	1.08792	4,4',8,27
B	10	3.05448	1.37703	0.15415	1.05905	11,29,29',33
C	14	4.39587	1.60413	0.70711	1.02157	12,12',16,16',33



	X	Y	Z
1	0.00000	0.00000	0.70711
2	1.00000	0.00000	0.70711
3	-0.50000	0.50000	0.00000
4	0.50000	0.50000	0.00000
5	1.50000	0.50000	0.00000
6	1.00000	1.00000	0.70711
7	2.00000	1.00000	0.70711
8	3.00000	1.00000	0.70711
9	2.50000	1.50000	0.00000
10	3.50000	1.50000	0.00000
11	4.50000	1.50000	0.00000
12	3.00000	2.00000	0.70711
13	4.00000	2.00000	0.70711
14	5.00000	2.00000	0.70711
15	6.00000	2.00000	0.70711
16	4.50000	2.50000	0.00000
17	5.50000	2.50000	0.00000
18	6.50000	2.50000	0.00000
19	6.00000	3.00000	0.70711
20	-0.89017	1.10963	0.72410
21	-0.16607	1.79933	0.72410
22	0.55813	2.48893	0.72410
23	1.28223	3.17863	0.72410
24	2.00643	3.86823	0.72410
25	0.54083	1.78213	0.01699
26	1.26493	2.47183	0.01699
27	1.98913	3.16143	0.01699
28	2.71323	3.85113	0.01699
29	1.97183	2.45463	0.72410
30	2.69593	3.14433	0.72410
31	3.42013	3.83393	0.72410
32	3.40283	3.12713	0.01699
33	4.12693	3.81683	0.01699
34	4.85113	4.50643	0.01699
35	4.10983	3.10963	0.72410
36	4.83393	3.79933	0.72410
37	5.55813	4.48893	0.72410
38	5.54083	3.78213	0.01699
39	6.26493	4.47183	0.01699
40	1.50000	1.50000	0.0

[100] $\Sigma 29a$ 46.40° (073) $\Delta Z = 0.01699$

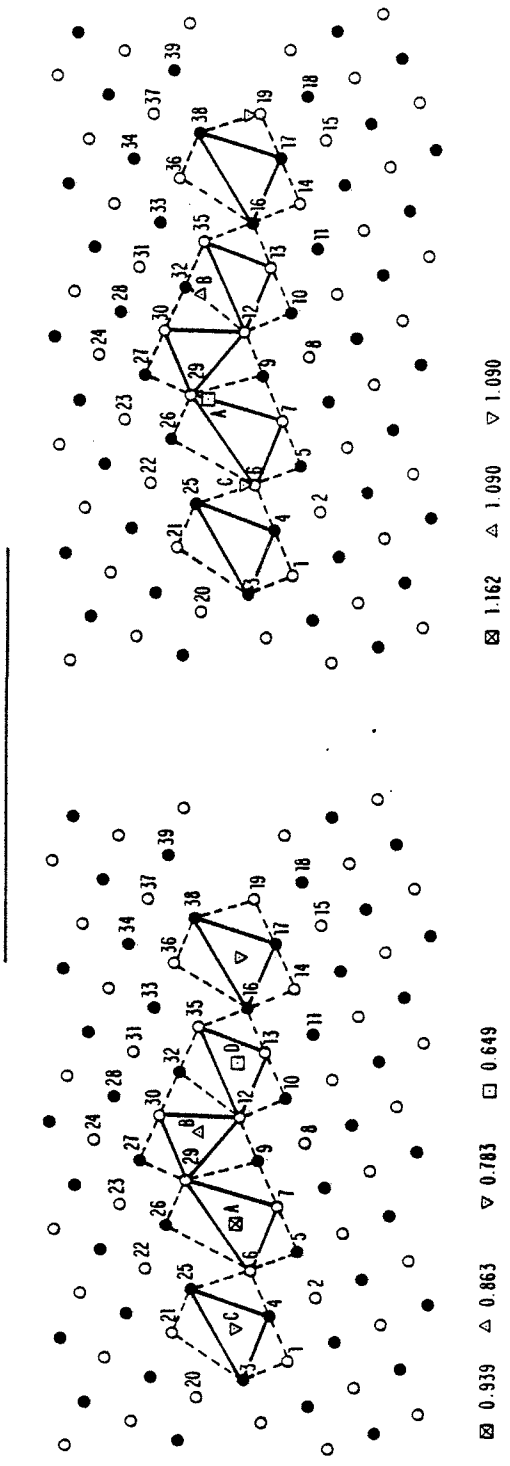
$v^{EX} = 0.48540$

Third densest

Contacts: 40-26, 40-25, 16-35

Interstitials	x	y	z	d	Touching
A	2.66375	2.51284	0.0	0.87197	12,12',27,30
B	0.08477	0.91523	0.70711	0.83830	1,4,4',6,21
C	1.23512	1.93806	0.70711	0.74592	40,40',22,26
D	4.82184	3.30216	0.01699	0.72896	16,36,36',38
E	3.67311	2.32689	0.0	0.68964	10,13,13',16,32
(F)	3.39281	2.71682	0.72412	0.63513	12,30,32,32',35
(G)	2.0	2.10852	0.01699	0.57554	9,40,29,29'
(H)	2.26714	1.73286	0.70711	0.56006	7,9,9',12,29
(I)	0.53573	1.57274	0.72410	0.47495	6,21,25,25'
(J)	0.86995	1.1046	0.0	0.46126	4,6,6',40,25
(K)	4.55508	2.55508	0.70711	0.42277	14,16,16',35

Substitutionals		x	y	z	d	Touching
A	32	3.39307	2.72738	0.01699	1.15393	12,30,30',35,35'
B	29	1.96191	2.13829	0.72409	1.09479	12,40,26,26'
C	12	2.96107	2.11679	0.70711	1.09095	9,9',13,29
(D)	6	0.87963	1.12037	0.70711	1.02877	4,4',40,40',25
(E)	25	0.49528	1.52875	0.01699	1.01056	6,40,21,21'



	X	Y	Z
1	0.00000	0.00000	0.70711
2	1.0	0.0	0.70711
3	-0.5	0.5	0.0
4	0.5	0.5	0.0
5	1.5	0.5	0.0
6	1.0	1.0	0.70711
7	2.0	1.0	0.70711
8	3.0	1.0	0.70711
9	2.5	1.5	0.0
10	3.5	1.5	0.0
11	4.5	1.5	0.0
12	3.0	2.0	0.70711
13	4.0	2.0	0.70711
14	5.0	2.0	0.70711
15	6.0	2.0	0.70711
16	4.5	2.5	0.0
17	5.5	2.5	0.0
18	6.5	2.5	0.0
19	6.0	3.0	0.70711
20	-1.0	1.0	0.70711
21	-0.2759	1.6897	0.70711
22	0.4483	2.3793	0.70711
23	1.1724	3.0690	0.70711
24	1.8966	3.7586	0.70711
25	0.4310	1.6725	0.0
26	1.1551	2.3622	0.0
27	1.8793	3.0518	0.0
28	2.6034	3.7415	0.0
29	1.8620	2.3450	0.70711
30	2.5861	3.0347	0.70711
31	3.3103	3.7243	0.70711
32	3.2930	3.0175	0.0
33	4.0171	3.7072	0.0
34	4.7413	4.3968	0.0
35	4.0	3.0	0.70711
36	4.7241	3.6897	0.70711
37	5.4483	4.3793	0.70711
38	5.4310	3.6725	0.0
39	6.1551	4.3622	0.0

[100] $\Sigma 29a$ 46.40° (073) $\Delta Z = 0$

$v^{EX} = 0.5211$

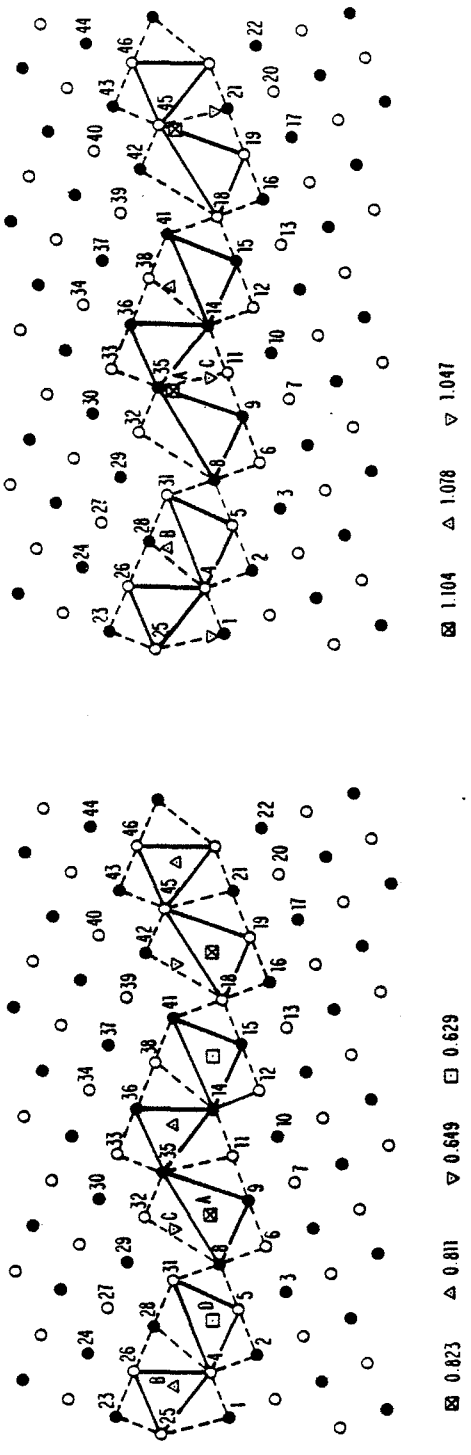
Fourth densest

Contacts: 13-35, 16-35, 16-35'

Interstitials	x	y	z	d	Touching
A	1.53118	1.46882	0.0	0.93863	5,7,7',9,26
B	2.57145	2.42865	0.0	0.86268	9,12,12',27,30,30',32
C	0.11401	0.88599	0.70711	0.78659	1,4,4',6,21
D	3.69987	2.30013	0.0	0.64943	10,13,13',16,32
(E)	4.71428	3.28573	0.0	0.62885	16,36,36',38
(F)	1.00006	1.80001	0.56563	0.62485	6,22,25,26
(G)	3.28562	2.71439	0.70711	0.53873	12,30,32,32',35
(H)	2.29060	1.70940	0.70711	0.53322	7,9,9',12,29

Substitutionals		x	y	z	d	Touching
A	29	1.92183	2.07817	0.70711	1.16199	7,9,9',12,26,26'
B	32	3.28562	2.71438	0.0	1.08990	12,12',30,30',35,35'
C	6	0.96152	1.11544	0.70711	1.08975	4,4',7,25,25'
(D)	9	0.46489	1.53510	0.0	1.07140	4,6,6',21,21'
(E)	26	1.46665	1.60005	0.0	1.07636	6,6',9,25
(F)	25	0.48132	1.59547	0.0	1.08688	6,6',21,21',26
(G)	12	2.97323	2.08032	0.70711	1.05982	9,9',13,30
(H)	36	5.0	3.10261	0.70711	1.01050	19,35,38,38'

Lattices exactly on the coincidence lattice; CSL sites: 20,35



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.0	0.0	0.0
3	2.0	0.0	0.0
4	0.5	0.5	0.70711
5	1.5	0.5	0.70711
6	2.5	0.5	0.70711
7	3.5	0.5	0.70711
8	2.0	1.0	0.0
9	3.0	1.0	0.0
10	4.0	1.0	0.0
11	3.5	1.5	0.70711
12	4.5	1.5	0.70711
13	5.5	1.5	0.70711
14	4.0	2.0	0.
15	5.0	2.0	0.0
16	6.0	2.0	0.0
17	7.0	2.0	0.0
18	5.5	2.5	0.70711
19	6.5	2.5	0.70711
20	7.5	2.5	0.70711
21	7.0	3.0	0.0
22	8.0	3.0	0.0
23	-0.6207	1.4484	0.0
24	0.0690	2.1725	0.0
25	-0.6035	0.7415	0.70711
26	0.0862	1.4656	0.70711
27	0.7759	2.1897	0.70711
28	0.7931	1.4828	0.0
29	1.4128	2.2069	0.0
30	2.1724	2.9311	0.0
31	1.5	1.5	0.70711
32	2.1897	2.2241	0.70711
33	2.8793	2.9483	0.70711
34	3.5690	3.6724	0.70711
35	2.8966	2.2413	0.0
36	3.5863	2.9654	0.0
37	4.2759	3.6896	0.0
38	4.2932	2.9826	0.70711
39	4.9829	3.7067	0.70711
40	5.6725	4.4309	0.70711
41	5.0	3.0	0.0
42	5.6897	3.7241	0.0
43	6.3793	4.4483	0.0
44	7.0690	5.1724	0.0
45	6.3966	3.7413	0.70711
46	7.0863	4.4654	0.70711

[100] $\Sigma 29a$ 43.60° (052) $\Delta z = 0$

$v^{EX} = 0.4422$

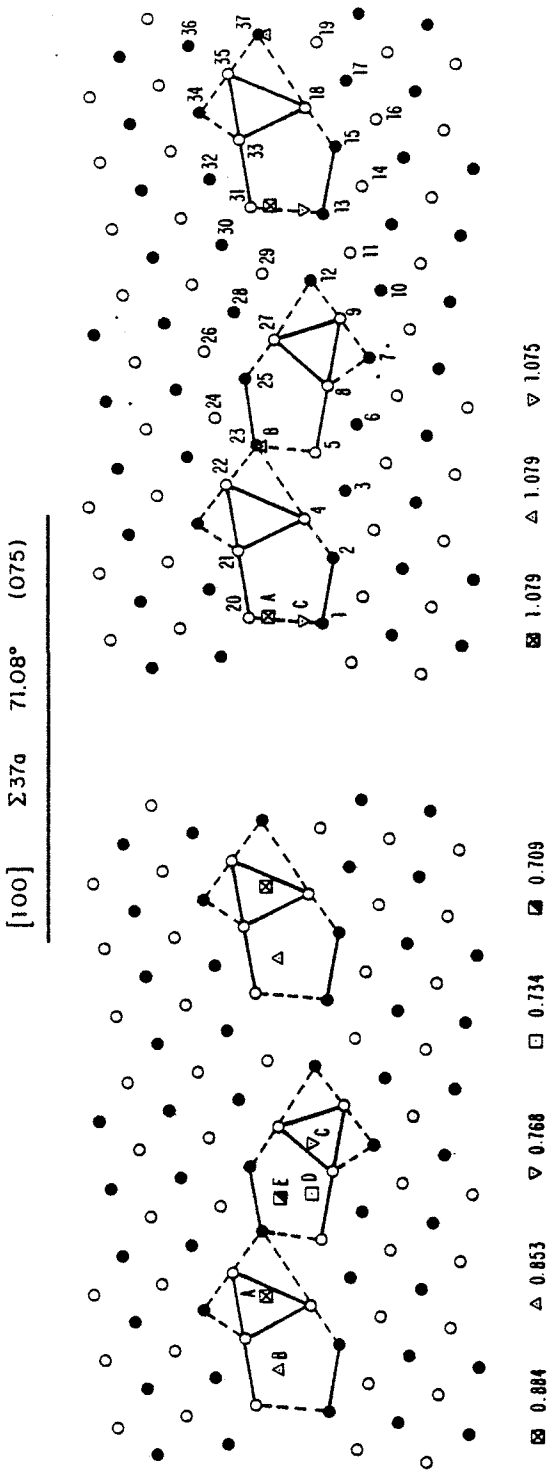
Not the densest

Contacts: 5-31, 8-31, 8-31'

Interstitials	x	y	z	d	Touching
A	2.59324	1.40676	0.70711	0.82307	6,9,9',11,32
B	0.09996	0.90000	0.0	0.81114	1,4,4',23,26,26',28
C	2.2	1.8	0.0	0.64922	8,29,32,32',35
D	1.21427	0.78573	0.0	0.62885	2,5,5',8,28
(E)	0.8	1.2	0.70711	0.52317	4,26,28,28',31
(F)	3.34620	1.65380	0.0	0.47960	9,11,11',14,35

Substitutionals		x	y	z	d	Touching
A	35	2.94917	2.05083	0.0	1.10411	9,11,11',14,32,32'
B	28	0.8	1.2	0.0	1.07847	4,4',26,26',31,31'
C	11	3.34621	1.65380	0.70711	1.04676	9,9',14,14',35,35'
(D)	4	0.48798	0.53606	0.70711	1.02532	1,1',5,26
(E)	32	2.5	1.63950	0.70711	1.01937	11,31,35,35'

Lattices exactly on the coincidence lattice; CSL sites: 31,41



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	2.00000	0.00000	0.00000
4	1.50000	0.50000	0.70711
5	2.50000	0.50000	0.70711
6	3.00000	0.00000	0.00000
7	4.00000	0.00000	0.00000
8	3.50000	0.50000	0.70711
9	4.50000	0.50000	0.70711
10	5.00000	0.00000	0.00000
11	5.50000	0.50000	0.70711
12	5.00000	1.00000	0.00000
13	6.00000	1.00000	0.00000
14	6.50000	0.50000	0.70711
15	7.00000	1.00000	0.00000
16	7.50000	0.50000	0.70711
17	8.00000	1.00000	0.00000
18	7.50000	1.50000	0.70711
19	8.50000	1.50000	0.70711
20	-0.07869	1.03101	0.70711
21	0.86726	1.35533	0.70711
22	1.81320	1.67966	0.70711
23	2.44834	1.36885	0.00000
24	2.75915	2.00398	0.70711
25	3.39428	1.69317	0.00000
26	3.70509	2.32831	0.70711
27	4.02942	1.38236	0.70711
28	4.34023	2.01750	0.00000
29	4.97536	1.70669	0.70711
30	5.28618	2.34182	0.00000
31	5.92131	2.03101	0.70711
32	6.23212	2.66615	0.00000
33	6.86726	2.35534	0.70711
34	7.17807	2.99047	0.00000
35	7.81320	2.67966	0.70711
36	8.12401	3.31480	0.00000
37	8.44834	2.36885	0.00000

[100] $\Sigma 37a$ 71.08° (075) $\Delta Z = 0$

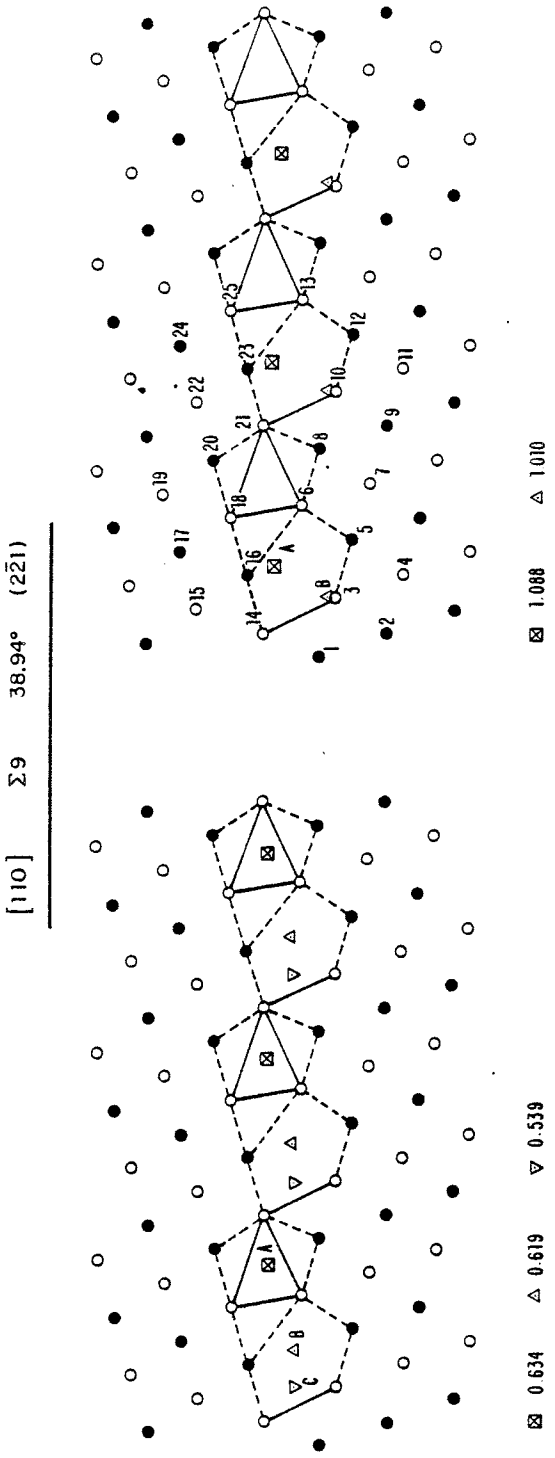
$v^{EX} = 0.51018$

Not the densest

Contacts: 9-27, 12-29, 12-29'

Interstitials	x	y	z	d	Touching
A	1.53975	1.12085	0.0	0.88365	4,4',22,22',23,unnumbered also at 18,18',34,35,35',37
B	0.5	0.77959	0.02853	0.85318	13,15,31,32
C	3.87500	0.87500	0.0	0.76777	7,8,8',27,27'
D	3.15108	0.86083	0.0	0.73429	8,8',23,25
E	3.0	1.18816	0.62691	0.70880	5,8,23,24
(F)	6.29884	1.29884	0.70711	0.64755	13,13',14,31
(G)	5.64942	1.28236	0.65886	0.59591	11,13,29,31
(H)	5.5	1.59479	0.13011	0.57569	12,13,29,30
(I)	2.0	0.99866	0.46712	0.49165	4,5,22,23

Substitutionals		x	y	z	d	Touching
A	20	0.01353	0.76203	0.70711	1.07930	13,13',29,33
B	23	2.44926	1.26022	0.0	1.07895	5,5',22,22',25
C	1	0.0	0.27603	0.0	1.07479	12,15,31,31'
(D)	4	1.48429	0.54714	0.70711	1.03361	2,2',5,21
(E)	15	6.78827	1.63520	0.0	1.02469	13,18,18',33,33'
(F)	5	2.5	0.64822	0.70711	1.02185	4,8,23,23'
(G)	33	6.88835	2.29380	0.66111	1.00634	18,31,32,34,35
(H)	8	3.50000	0.53335	0.68353	1.00167	5,6,7,9,27



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.0	0.0	0.0
3	0.5	0.70711	0.5
4	1.5	0.70711	0.5
5	1.0	1.41421	0.0
6	0.5	2.12132	0.5
7	1.5	2.12132	0.5
8	1.0	2.82843	0.0
9	2.0	2.82843	0.0
10	1.5	3.53553	0.5
11	2.5	3.53553	0.5
12	2.0	4.24264	0.0
13	1.5	4.94975	0.5
14	-0.57907	0.64395	0.5
15	-1.35685	1.27250	0.5
16	-0.52351	1.50820	0.0
17	-1.30129	2.13674	0.0
18	-0.46796	2.37244	0.5
19	-1.24574	3.00098	0.5
20	-0.41240	3.23668	0.0
21	0.42093	3.47238	0.5
22	-0.35685	4.10092	0.5
23	0.47649	4.33662	0.0
24	-0.30129	4.96516	0.0
25	0.53204	5.20086	0.5

[110] Σ9 38.94° $(2\bar{2}1)$ ΔZ = 0.0

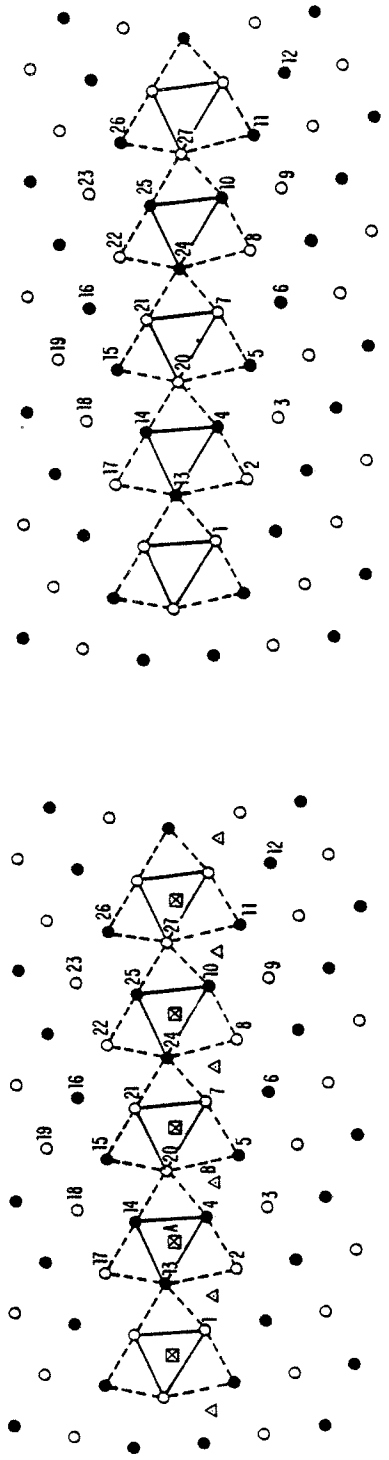
$v^{EX} = 0.3246$

Not the densest

Contacts: 6-18, 8-21, 8'-21

Interstitials	x	y	z	d	Touching
A	0.19495	2.69057	0.0	0.63354	6,6',8,20
B	0.10606	1.41421	0.5	0.61887	3,6,16,16'
C	-0.05262	0.89939	0.0	0.53933	3,3',14,14',16
(D)	-0.03367	2.05524	0.0	0.46860	6,6',16,18,18'

Substitutionals		x	y	z	d	Touching
A	16	-0.18132	1.48619	0.0	1.11431	6,6',14,14',16',16",18,18'
B	3	0.41861	0.76466	0.5	1.00991	1,1',3',3",5,5',14



	X	Y	Z
1	0.00000	0.00000	0.50000
2	1.0	0.0	0.5
3	2.0	0.0	0.5
4	1.5	0.70711	0.0
5	2.5	0.70711	0.0
6	3.5	0.70711	0.0
7	3.0	1.41421	0.5
8	4.0	1.41421	0.5
9	5.0	1.41421	0.5
10	4.5	2.12132	0.0
11	5.5	2.12132	0.
12	6.5	2.12132	0.
13	0.349	0.793	0.
14	0.985	1.564	0.
15	1.622	2.335	0.
16	2.258	3.107	0.
17	0.121	1.628	0.5
18	0.757	2.399	0.5
19	1.394	3.171	0.5
20	1.849	1.500	0.5
21	2.485	2.271	0.5
22	3.122	3.043	0.5
23	3.758	3.814	0.5
24	3.349	2.207	0.0
25	3.985	2.978	0.0
26	4.622	3.750	0.0
27	4.849	2.914	0.5

[110] Σ11 129.52° $(1\bar{1}3)$ $\Delta Z = 0.0$

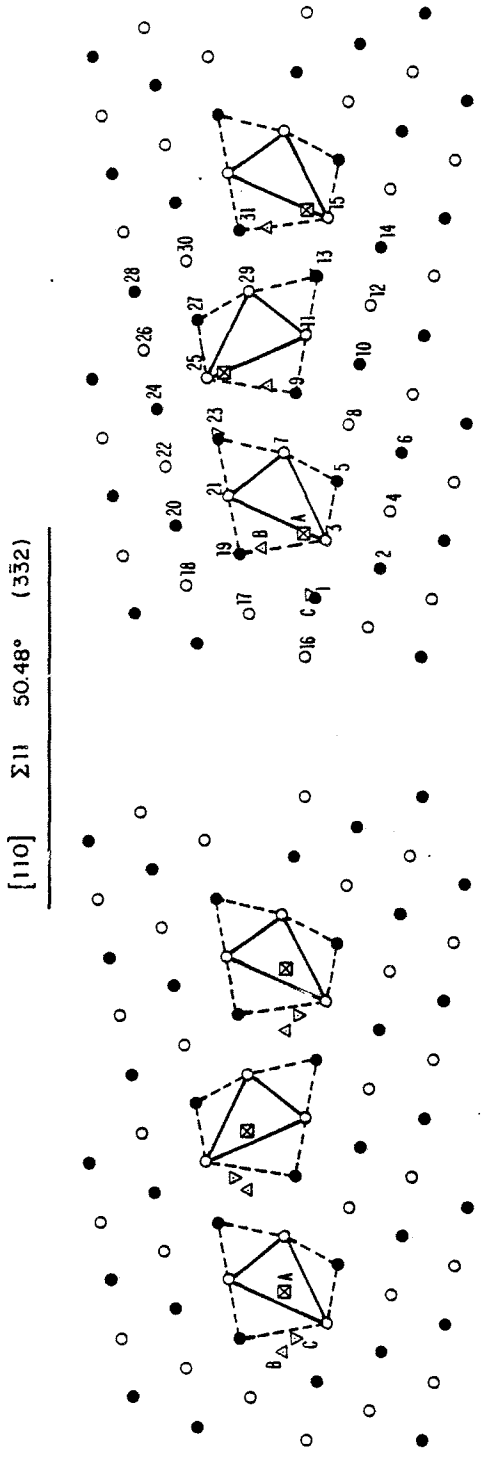
$v^{EX} = 0.1591$

Not the densest

Contacts: 4-14, 4-20, 4-20'

Interstitials	x	y	z	d	Touching
A	0.93968	0.95356	0.5	0.58074	4,4',13,13',14,14'
B	2.0	0.80263	0.5	0.42716	4,4',5,5',20

Substitutionals none > 1.0



	X	Y	Z
1	0.50000	0.70711	0.00000
2	1.5	0.70711	0.0
3	1.0	1.41421	0.5
4	2.0	1.41421	0.5
5	1.5	2.12132	0.0
6	2.5	2.12132	0.0
7	1.0	2.82842	0.5
8	2.0	2.82842	0.5
9	1.5	3.5355	0.0
10	2.5	3.5355	0.0
11	2.0	4.2426	0.5
12	3.0	4.2426	0.5
13	2.5	4.9497	0.0
14	3.5	4.9497	0.0
15	3.0	5.6569	0.5
16	0.0	0.0	0.5
17	-0.4226	0.9063	0.5
18	-1.0589	1.6777	0.5
19	-0.1953	1.7420	0.0
20	-0.8316	2.5134	0.0
21	0.0320	2.5776	0.5
22	-0.6043	3.3492	0.5
23	0.2593	3.4135	0.0
24	-0.3770	4.1849	0.0
25	0.4866	4.2493	0.5
26	-0.1497	5.0207	0.5
27	0.7139	5.0850	0.0
28	0.0776	5.8564	0.0
29	1.5776	5.1493	0.5
30	0.9413	5.9207	0.5
31	1.8049	5.9850	0.0

[110] $\Sigma 11$ 50.48° $(3\bar{3}2)$ $\Delta Z = 0.0$

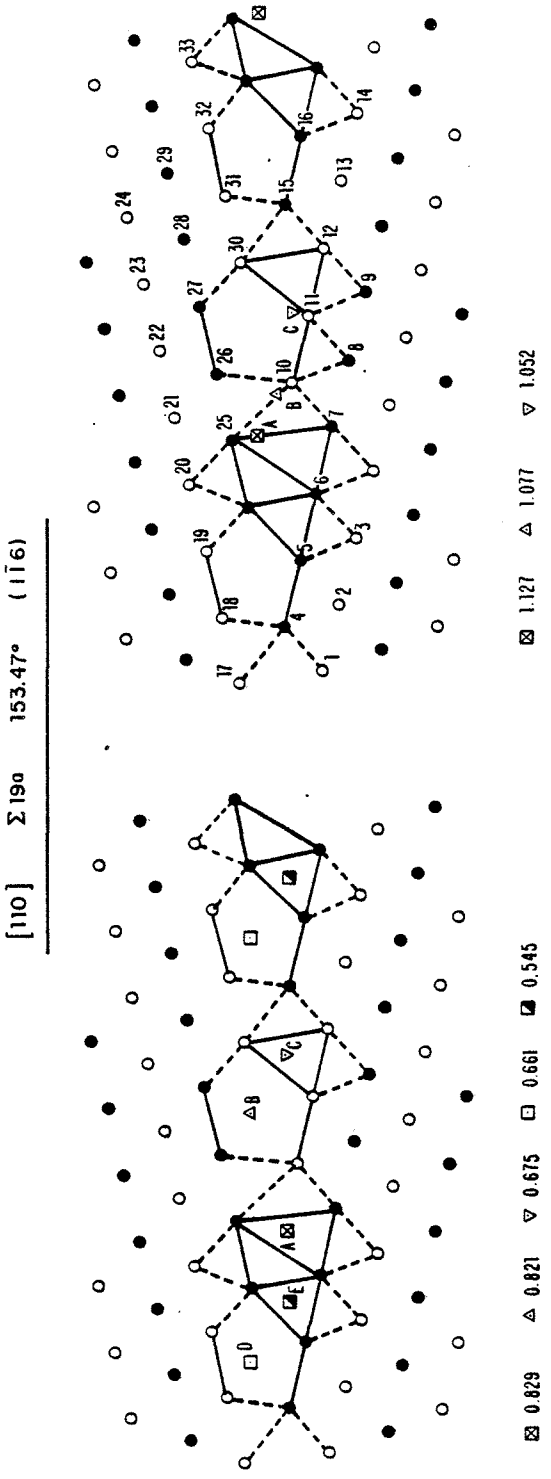
$V^{EX} = 0.3551$

Not the densest

Contacts: 7-21, 11-29

Interstitials	x	y	z	d	Touching
A	0.60993	2.12127	0.0	0.78015	5,19,21,21'
B	0.22902	1.32740	0.5	0.55170	3,17,19,19'
C	0.46816	1.43673	0.0	0.46063	1,3,3',19
(D)	0.50423	2.74852	0.0	0.41730	7,7',21,21',23

Substitutionals		x	y	z	d	Touching
A	19	0.72455	1.60899	0.5	1.11074	1,1',3',3",5,5',19,19'
B	3	0.08847	1.66476	0.0	1.08467	1,17,17',19',19",21,21'
C	1	0.43377	0.75394	0.0	1.00657	1',1",3,3',16,16',17,17'



	X	Y	Z
1	0.00000	0.00000	0.50000
2	1.00000	0.00000	0.50000
3	2.00000	0.00000	0.50000
4	0.50000	0.70711	0.00000
5	1.50000	0.70711	0.00000
6	2.50000	0.70711	0.00000
7	3.50000	0.70711	0.00000
8	4.50000	0.70711	0.00000
9	5.50000	0.70711	0.00000
10	4.00000	1.41421	0.50000
11	5.00000	1.41421	0.50000
12	6.00000	1.41421	0.50000
13	7.00000	1.41421	0.50000
14	8.00000	1.41421	0.50000
15	6.50000	2.12132	0.00000
16	7.50000	2.12132	0.00000
17	-0.49408	1.12029	0.50000
18	0.40092	1.56729	0.50000
19	1.29492	2.01329	0.50000
20	2.18992	2.46029	0.50000
21	3.08492	2.90729	0.50000
22	3.97992	3.35329	0.50000
23	4.87392	3.80029	0.50000
24	5.76892	4.24729	0.50000
25	2.95392	2.05129	0.00000
26	3.84892	2.49829	0.00000
27	4.74292	2.94429	0.00000
28	5.63792	3.39129	0.00000
29	6.53292	3.83829	0.00000
30	5.50692	2.53529	0.50000
31	6.40192	2.98229	0.50000
32	7.29592	3.42829	0.50000
33	-0.36308	1.97629	0.00000
34	0.53192	2.42329	0.00000
35	2.05918	1.60470	0.00000

[110] Σ19a 153.47° $(1\bar{1}6)$ $\Delta Z = 0.0$

$v^{EX} = 0.44981$

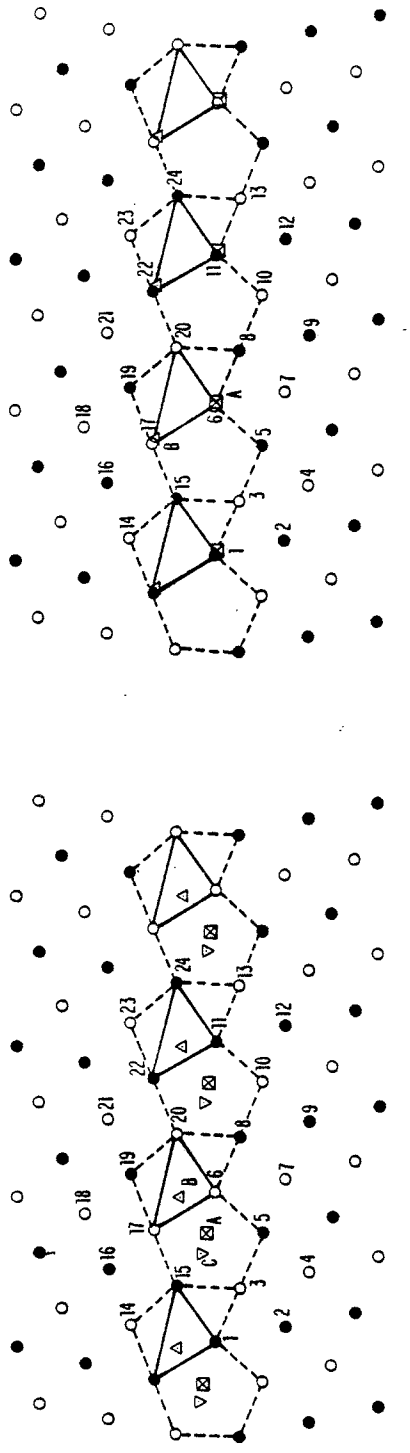
Not the densest

Contacts: 6-32, 15-31, 15-31'

Interstitials	x	y	z	d	Touching
A	3.0	1.28700	0.5	0.82895	6,6',7,7',25,25'
B	4.55232	2.20733	0.5	0.82148	11,26,26',27,27'
C	5.5	1.86327	0.0	0.67530	11,11',12,12',30,30'
D	1.04254	1.40017	0.0	0.66085	5,18,18',19,19'
E	2.0	1.01859	0.5	0.54534	5,5',6,6',32,32'
(F)	3.53035	2.01663	0.5	0.52771	10,25,25',26,26'
(G)	3.43182	1.46243	0.0	0.51677	7,10,10',25
(H)	0.00940	1.23171	0.0	0.43653	4,17,17',18,18'

Substitutionals		x	y	z	d	Touching
A	25	3.11573	1.72824	0.0	1.12655	10,10',25',25",26,32
B	10	3.74384	1.58919	0.49128	1.07737	7,10',25,26
C	11	5.0	1.64336	0.5	1.05184	10,11',11",12,30
(D)	30	5.50002	2.30928	0.5	1.05049	11,12,30',30"
(E)	26	3.94473	2.30485	0.0	1.04548	10,10',25,26',26",27
(F)	5	1.5	0.77304	0.0	1.00434	4,5',5",6,32

[110] Σ19a 26.53° (3$\bar{3}$1)



⊠ 0.625 △ 0.485 ▽ 0.463

⊠ 1.0003 △ 1.0003

	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.0	0.0	0.0
3	0.5	0.70711	0.5
4	1.5	0.70711	0.5
5	1.0	1.41421	0.0
6	0.5	2.12132	0.5
7	1.5	2.12132	0.5
8	1.0	2.82843	0.0
9	2.0	2.82843	0.0
10	1.5	3.53553	0.5
11	1.0	4.24264	0.0
12	2.0	4.24264	0.0
13	1.5	4.94975	0.5
14	-1.09649	0.53343	0.5
15	-0.33333	0.94281	0.0
16	-1.22807	1.38940	0.0
17	-0.46491	1.79878	0.5
18	-1.35965	2.24537	0.5
19	-0.59649	2.65475	0.0
20	0.16667	3.06413	0.5
21	-0.72807	3.51072	0.5
22	0.03509	3.92010	0.0
23	-0.09649	4.77607	0.5
24	0.66667	5.18545	0.0

[110] Σ19a 26.53° $(3\bar{3}1)$ $\Delta Z = 0.0$

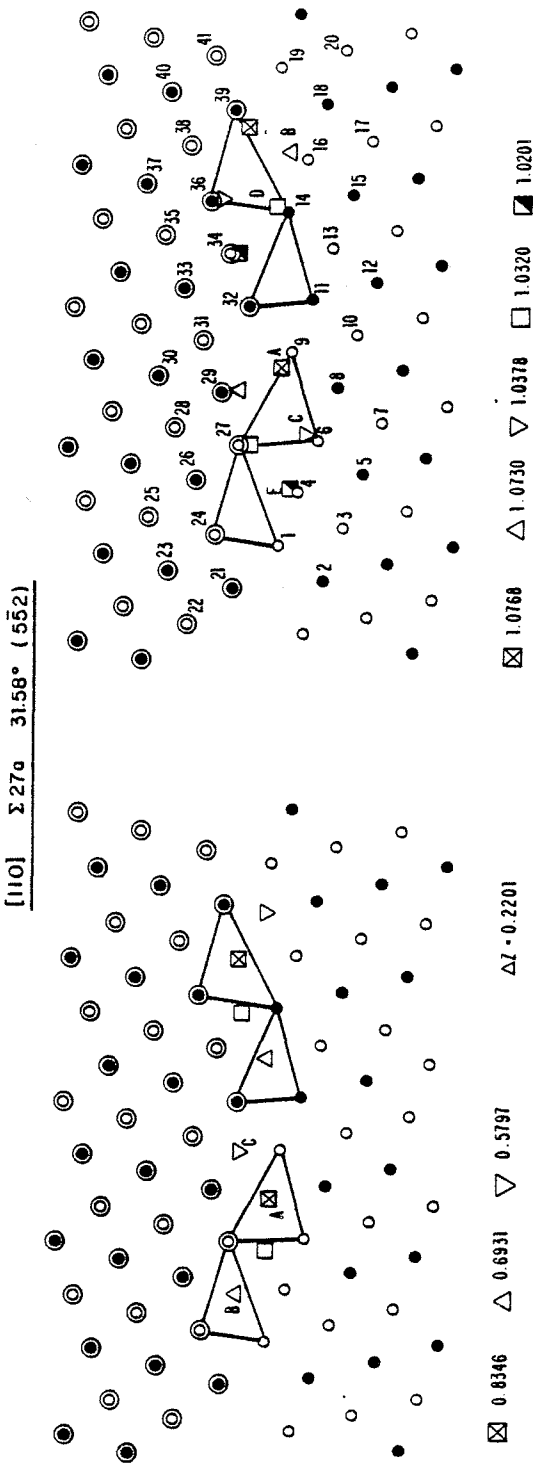
$V^{EX} = 0.2428$

Not the densest

Contacts: 1-15, 3-15, 3'-15

Interstitials		x	y	z	d	Touching
	A	0.2	1.55564	0.0	0.62480	5,6,6',15
	B	-0.04762	2.15500	0.0	0.48463	6,6',17,17',19
	C	0.06664	1.29633	0.5	0.46283	3,15,15',17 (Not a stable site)

Substitutionals		x	y	z	d	Touching
A	6	0.48530	2.11092	0.5	1.00032	5,5',6',6",17
B	17	-0.44760	1.80144	0.5	1.00030	6,15,15',17',17",19,19'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	-0.70711	0.50000
3	1.00000	0.00000	0.00000
4	0.50000	0.70711	0.50000
5	1.50000	0.70711	0.50000
6	1.00000	1.41421	0.00000
7	2.00000	1.41421	0.00000
8	1.50000	2.12132	0.50000
9	1.00000	2.82843	0.00000
10	2.00000	2.82843	0.00000
11	1.50000	3.53553	0.50000
12	2.50000	3.53553	0.50000
13	2.00000	4.24264	0.00000
14	1.50000	4.94975	0.50000
15	2.50000	4.94975	0.50000
16	2.00000	5.65685	0.00000
17	3.00000	5.65685	0.00000
18	2.50000	6.36396	0.50000
19	2.00000	7.07107	0.00000
20	3.00000	7.07107	0.00000
21	-0.83688	-0.47040	0.27991
22	-1.63318	-0.81086	0.77991
23	-1.68874	0.05338	0.27991
24	-0.89244	0.39384	0.77991
25	-1.74429	0.91762	0.77991
26	-0.94800	1.25808	0.27991
27	-0.15170	1.59854	0.77991
28	-1.00355	2.12233	0.77991
29	-0.20725	2.46278	0.27991
30	-1.05911	2.98657	0.27991
31	-0.26281	3.32703	0.77991
32	0.53349	3.66749	0.27991
33	-0.31837	4.19127	0.27991
34	0.47793	4.53173	0.77991
35	-0.37392	5.05551	0.77991
36	0.42237	5.39597	0.27991
37	-0.42948	5.91975	0.27991
38	0.36682	6.26021	0.77991
39	1.16312	6.60067	0.27991
40	0.31126	7.12445	0.27991
41	1.10756	7.46491	0.77991

[110] Σ27a 31.58° $(5\bar{5}2)$ $\Delta Z = 0.22009$

Symmetrical

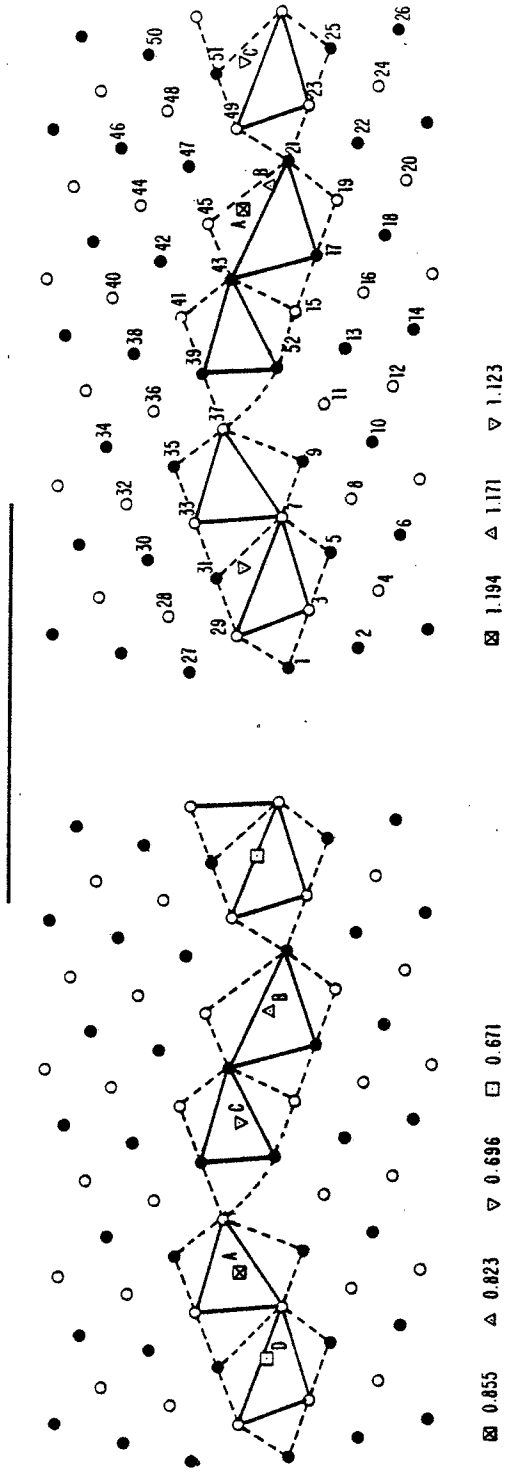
$V^{EX} = 0.43619$

Second densest

Contacts: 1-24, 1-21, 9-32, 11-32

Interstitials	x	y	z	d	Touching
A	0.58685	2.12132	0.58685	0.83455	6,8,9,29
B	-0.24172	0.82381	0.10901	0.69313	4,24,26,27
C	0.37511	2.93478	0.52878	0.57972	9,29,31,32
D	0.32929	1.37931	0.27991	0.45522	4,8,27,27'

Substitutionals		x	y	z	d	Touching
A	9	0.77163	2.66694	0.0	1.07676	8,8',9',9'',29
B	16	1.77746	5.81421	0.0	1.07295	14,14',16',16'',18,18',39
C	6	0.84055	1.52696	0.0	1.03778	4,4',6',6'',8,8',27
D	14	1.35327	5.05350	0.5	1.03204	14',14'',16,16',36
E	4	0.38389	0.78921	0.5	1.02012	1,1',4',4'',6,6',27



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	0.50000	0.70711	0.50000
4	1.50000	0.70711	0.50000
5	1.00000	1.41421	0.00000
6	2.00000	1.41421	0.00000
7	0.50000	2.12132	0.50000
8	1.50000	2.12132	0.50000
9	1.00000	2.82843	0.00000
10	2.00000	2.82843	0.00000
11	1.50000	3.53553	0.50000
12	2.50000	3.53553	0.50000
13	2.00000	4.24264	0.00000
14	3.00000	4.24264	0.00000
15	1.50000	4.94975	0.50000
16	2.50000	4.94975	0.50000
17	2.00000	5.65685	0.00000
18	3.00000	5.65685	0.00000
19	2.50000	6.36396	0.50000
20	3.50000	6.36396	0.50000
21	2.00000	7.07107	0.00000
22	3.00000	7.07107	0.00000
23	2.50000	7.77817	0.50000
24	3.50000	7.77817	0.50000
25	3.00000	8.48528	0.00000
26	4.00000	8.48528	0.00000
27	-1.34320	0.33130	0.00000
28	-1.39920	1.19530	0.50000
29	-0.54720	0.67141	0.50000
30	-1.45520	2.05930	0.00000
31	-0.60320	1.53530	0.00000
32	-1.51020	2.92330	0.50000
33	-0.65820	2.40030	0.50000
34	-1.56620	3.78830	0.00000
35	-0.71420	3.26430	0.00000
36	-0.77020	4.12830	0.50000
37	0.08180	3.60430	0.50000
38	-0.82520	4.99230	0.00000
39	0.02580	4.46830	0.00000
40	-0.88120	5.85630	0.50000
41	-0.02920	5.33230	0.50000
42	-0.08520	6.19730	0.00000
43	0.76680	5.67330	0.00000
44	-0.14120	7.06130	0.50000
45	0.71080	6.53730	0.50000
46	-0.19620	7.92530	0.00000
47	0.65580	7.40130	0.00000
48	0.59980	8.26630	0.50000
49	1.45280	7.74230	0.50000
50	0.54380	9.13030	0.00000
51	1.39580	8.60630	0.00000
52	1.00000	4.24264	0.00000

[110] $\Sigma 27a$ 31.58° $(5\bar{5}2)$ $\Delta Z = 0.0$

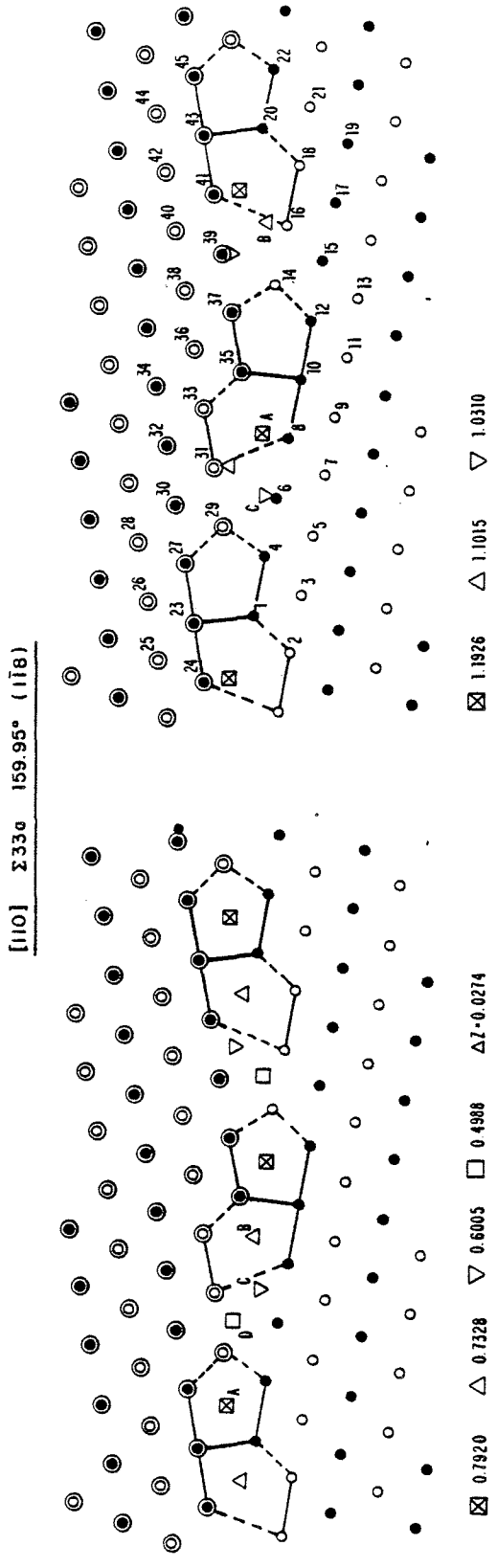
$V^{EX} = 0.47211$

Third densest

Contacts: 1-29, 1-29', 39-52

Interstitials	x	y	z	d	Touching
A	0.07415	2.77599	0.0	0.85467	7,7',9,35
B	1.59078	6.29976	0.5	0.82296	17,17',19,45
C	0.65937	4.83707	0.5	0.69632	15,41,52,52'
D	0.05506	1.41421	0.5	0.67089	3,7,31,31'
(E)	1.23543	6.85977	0.0	0.58647	21,45,45',47
(F)	-0.03397	0.99375	0.0	0.57137	3,3',29,29',31
(G)	0.67446	3.53553	0.0	0.55689	9,37,37',52
(H)	0.77964	3.33780	0.5	0.49400	9,9',11,37
(I)	0.96872	4.97188	0.0	0.45982	15,15',43,52
(J)	0.47886	4.20853	0.5	0.44603	37,39,39',52,52'

Substitutionals		x	y	z	d	Touching
A	45	1.16334	6.56634	0.49912	1.19443	21,43,45',47
B	21	1.63893	6.79674	0.0	1.17139	19,19',45,45',49,49'
C	31	2.17518	8.62968	0.0	1.12271	7,7',29,29',31',31",33,33'
(D)	37	0.40219	3.53553	0.5	1.10464	9,9',37',37",52,52'
(E)	9	0.76307	2.99597	0.0	1.08250	7,7',9',9",11,11',37,37'
(F)	7	0.28185	1.96706	0.5	1.07016	5,5',7',7",33
(G)	17	1.79071	5.80484	0.0	1.06466	15,15',17',17",19,19',43
(H)	43	0.97824	5.68679	0.0	1.04440	17,43',43",45,45'
(I)	33	-0.47438	2.41200	0.5	1.03364	7,31,31',33',33",35,35'
(J)	15	1.37504	5.03811	0.5	1.02329	15',15",17,17',43,43',52,52'
(K)	3	0.45210	0.74098	0.5	1.00344	1,1',3',3",5,5',29



	X	Y	Z
1	0.00000	0.00000	0.00000
2	-0.50000	-0.70711	0.50000
3	0.50000	-0.70711	0.50000
4	1.00000	-0.00000	0.00000
5	1.50000	-0.70711	0.50000
6	2.00000	0.00000	0.00000
7	2.50000	-0.70711	0.50000
8	3.00000	0.00000	0.00000
9	3.50000	-0.70711	0.50000
10	4.00000	0.00000	0.00000
11	4.50000	-0.70711	0.50000
12	5.00000	0.00000	0.00000
13	5.50000	-0.70711	0.50000
14	5.50000	0.70711	0.50000
15	6.00000	0.00000	0.00000
16	6.50000	0.70711	0.50000
17	7.00000	0.00000	0.00000
18	7.50000	0.70711	0.50000
19	8.00000	0.00000	0.00000
20	8.00000	1.41421	0.00000
21	8.50000	0.70711	0.50000
22	9.00000	1.41421	0.00000
23	-0.29392	0.95544	0.02736
24	-1.23332	0.61260	0.02736
25	-1.00605	1.44827	0.52736
26	-0.06665	1.79111	0.52736
27	0.64547	1.29828	0.02736
28	0.87274	2.13395	0.52736
29	1.35759	0.80544	0.52736
30	1.58486	1.64112	0.02736
31	2.29699	1.14828	0.52736
32	2.52426	1.98396	0.02736
33	3.23638	1.49112	0.52736
34	3.46365	2.32680	0.02736
35	3.94850	0.99829	0.02736
36	4.17577	1.83396	0.52736
37	4.88789	1.34113	0.02736
38	5.11517	2.17680	0.52736
39	5.82729	1.68397	0.02736
40	6.05456	2.51964	0.52736
41	6.76668	2.02681	0.02736
42	6.99396	2.86248	0.52736
43	7.70608	2.36965	0.02736
44	7.93335	3.20532	0.52736
45	8.64547	2.71249	0.02736

[110] Σ33a 159.95° $(1\bar{1}8)$ $\Delta z = 0.02736$

Symmetrical

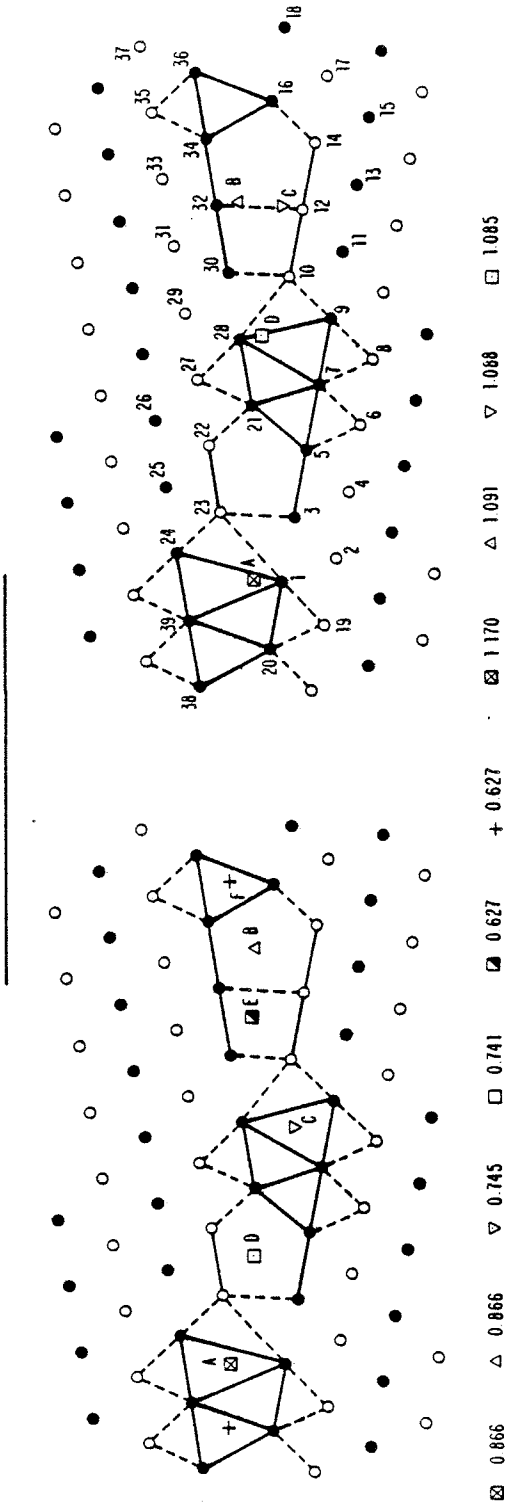
$v^{EX} = 0.42962$

Second densest

Contacts: 1-23, 4-29, 10-35, 14-37

Interstitials	x	y	z	d	Touching
A	0.49882	0.55135	0.5	0.79199	1,1',27,29
B	3.32301	0.62951	0.5	0.73277	8,8',33,35
C	2.5	0.37470	0.5	0.60050	6,6',8,8',31
D	1.91237	0.74374	0.02736	0.49878	6,29,29',31,31'
E	1.5	0.10539	0.5	0.42983	4,4',6,6',29
F	1.99984	0.50406	0.5	0.41996	6,6',29,31

Substitutionals		X	y	z	d	Touching
A	8	3.0	0.44926	0.0	1.19256	6,8',8'',10,35
B	16	6.5	1.02967	0.5	1.10147	14,16',16'',18,39
C	6	2.0	0.17681	0.0	1.03102	4,6',6'',8,30



	X	Y	Z
1	0.00000	0.00000	0.00000
2	0.50000	-0.70711	0.50000
3	1.00000	0.00000	0.00000
4	1.50000	-0.70711	0.50000
5	2.0000	0.00000	0.00000
6	2.50000	-0.70711	0.50000
7	3.00000	0.00000	0.00000
8	3.50000	-0.70711	0.50000
9	4.00000	0.00000	0.00000
10	4.50000	0.70711	0.50000
11	5.00000	0.00000	0.00000
12	5.50000	0.70711	0.50000
13	6.00000	0.00000	0.00000
14	6.50000	0.70711	0.50000
15	7.00000	0.00000	0.00000
16	7.00000	1.41421	0.00000
17	7.50000	0.70711	0.50000
18	8.00000	1.41421	0.00000
19	0.50000	-0.70711	0.50000
20	-1.00000	0.00000	0.00000
21	2.52993	0.88263	0.00000
22	1.81781	1.37546	0.50000
23	0.87841	1.03262	0.50000
24	0.16629	1.52545	0.00000
25	1.10569	1.86829	0.00000
26	2.04508	2.21113	0.00000
27	2.75720	1.71830	0.50000
28	2.46932	1.22547	0.00000
29	3.69660	2.06114	0.50000
30	4.40872	1.56831	0.00000
31	4.63599	2.40398	0.50000
32	5.34811	1.91115	0.00000
33	5.57538	2.74682	0.50000
34	6.28751	2.25399	0.00000
35	6.51478	3.08966	0.50000
36	7.22690	2.59683	0.00000
37	7.45417	3.43250	0.50000
38	-1.71249	0.83978	0.00000
39	-0.77310	1.52546	0.00000

[110] $\Sigma 33a$ 159.95° $(1\bar{1}8)$ $\Delta z = 0.0$

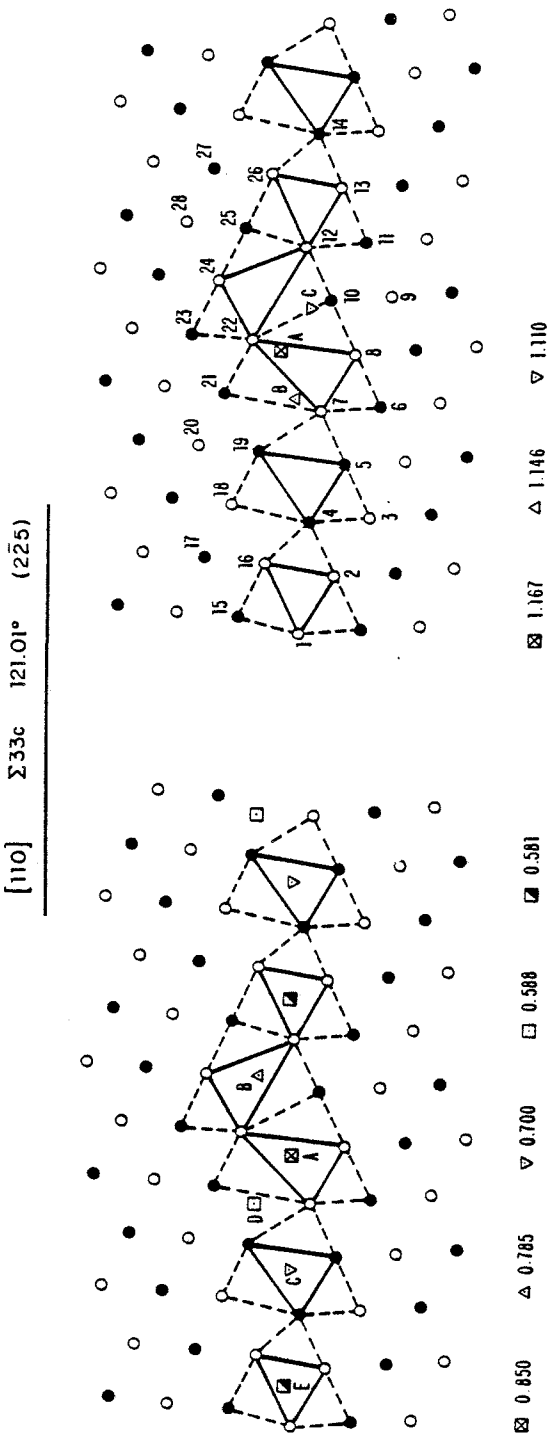
$V^{EX} = 0.48125$

Third densest

Contacts: 7-21, 10-30, 10'-30

Interstitials	x	y	z	d	Touching
A	7.90533	2.19632	0.5	0.86619	1,1',24,24',39,39'
B	6.02644	1.51091	0.5	0.86583	14,32,32',34,34'
C	3.5	0.51112	0.5	0.74498	7,7',9,9',28,28'
D	1.52207	0.72737	0.0	0.74067	5,22,22',23,23'
E	5.01644	1.36153	0.5	0.62737	12,30,30',32,32'
F	6.89516	2.04740	0.5	0.62717	16,16',34,34',36,36'
G	1.98835	0.60734	0.5	0.57353	5,5',21,21',22
H	0.5	0.34355	0.5	0.57229	1,1', 3,3',23
I	2.5	0.30020	0.5	0.53639	5,5',7,7',21,21'
J	3.99828	1.23452	0.5	0.45585	10,28,28',30,30'
K	3.98199	0.71984	0.0	0.44013	9,10,10',28

Substitutionals		x	y	z	d	Touching
A	1	0.0	0.42122	0.0	1.17018	1',1",3,20,39
B	32	5.45284	1.62421	0.0	1.09122	12,12',30,32',32",34
C	12	5.5	1.00726	0.5	1.08815	10,12',12",14,32,32'
D	28	3.57006	0.94946	0.0	1.08454	9,21,28',28",30
E	39	-0.69842	0.97800	0.0	1.04689	20,38,39',39",24
F	23	0.75762	0.85808	0.5	1.04456	3,3',23',23",24,24'
G	3	1.0	0.16032	0.0	1.02554	1,3',3",5,23,23'
H	16	7.0	1.54096	0.0	1.01600	16',16",18,34
I	34	6.32283	2.15721	0.0	1.01059	16,32,34',34",36
J	5	2.0	0.03391	0.0	1.00115	3,5',5",7,21



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	2.00000	0.00000	0.00000
4	1.50000	0.70711	0.50000
5	2.50000	0.70711	0.50000
6	3.50000	0.70711	0.50000
7	3.00000	1.41421	0.00000
8	4.00000	1.41421	0.00000
9	5.00000	1.41421	0.00000
10	4.50000	2.12132	0.50000
11	5.50000	2.12132	0.50000
12	5.00000	2.82843	0.00000
13	6.00000	2.82843	0.00000
14	6.50000	3.53553	0.50000
15	-0.19697	0.87853	0.50000
16	0.66667	0.94281	0.00000
17	0.31818	1.73563	0.50000
18	1.18182	1.79991	0.00000
19	2.04546	1.86419	0.50000
20	1.69697	2.65701	0.00000
21	2.56061	2.72129	0.50000
22	3.42424	2.78557	0.00000
23	3.07576	3.57839	0.50000
24	3.93939	3.64267	0.00000
25	4.80303	3.70696	0.50000
26	5.66667	3.77124	0.00000
27	5.31818	4.56405	0.50000
28	4.45455	4.49977	0.00000

[110] $\Sigma 33_C$ 121.01° $(2\bar{2}5)$ $\Delta Z = 0.0$

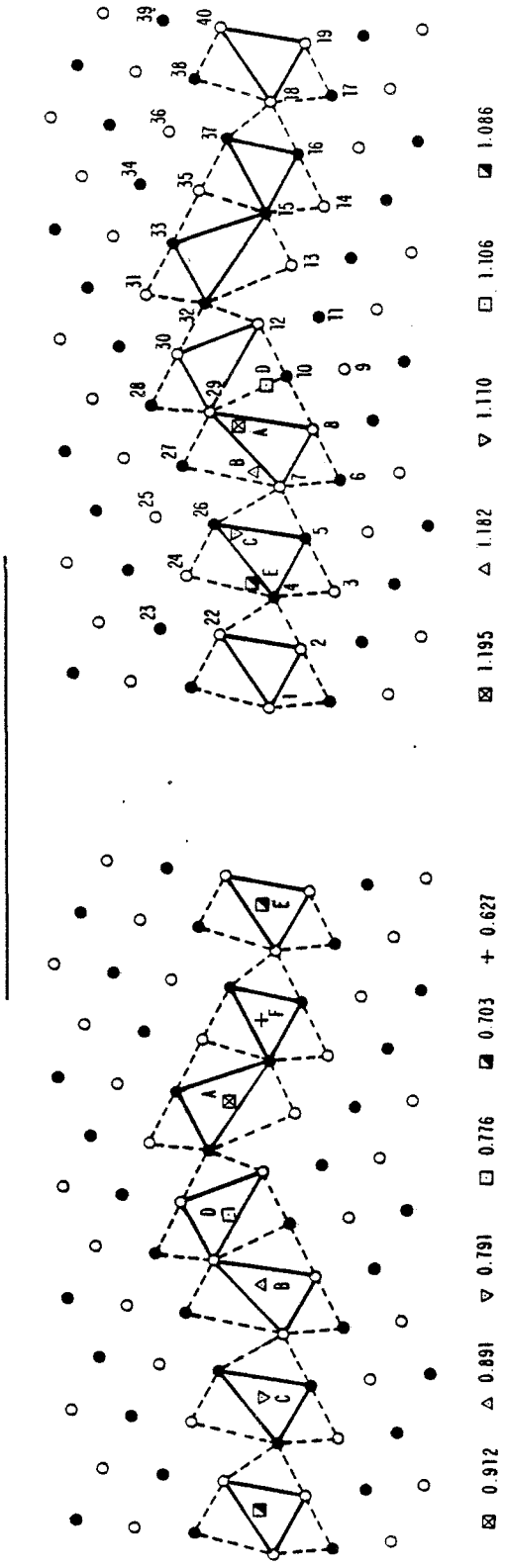
$V^{EX} = 0.41450$

Not the densest

Contacts: 2-16, 4-16, 4'-16

Interstitials	x	y	z	d	Touching
A	3.5	2.01083	0.5	0.85036	7,7',8,8',22,22'
B	4.27778	2.98557	0.5	0.78470	10,12,12',24,24',25
C	2.0	1.17851	0.0	0.69967	4,4',5,5',19,19'
D	2.61225	2.10689	0.0	0.58765	7,19,19',21,21'
E	0.5	0.35356	0.5	0.58114	1,1',2,2',16,16'
F	1.06410	1.28730	0.5	0.45138	4,16,16',18,18'

Substitutionals		x	y	z	d	Touching
A	22	3.5	2.37543	0.0	1.16698	7,8,22',22"
B	7	2.99286	1.80312	0.0	1.14597	7',7",19,19',22
C	10	4.22549	2.31543	0.5	1.11001	8,8',10',10",12,12',22,22'
D	19	2.06250	1.63520	0.5	1.05205	5,18,18',19',19"
E	4	1.53724	0.99672	0.5	1.01077	16,16',5,19
F	12	4.96296	2.85462	0.0	1.00206	10,10',12',12",25,25'
G	25	4.80555	3.67303	0.5	1.00116	12,12',24,24',25',25",26,26'



	X	Y	Z
1	0.00000	0.00000	0.00000
2	1.00000	0.00000	0.00000
3	2.00000	0.00000	0.00000
4	1.50000	0.70711	0.50000
5	2.50000	0.70711	0.50000
6	3.50000	0.70711	0.50000
7	3.00000	1.41421	0.00000
8	4.00000	1.41421	0.00000
9	5.00000	1.41421	0.00000
10	4.50000	2.12132	0.50000
11	5.50000	2.12132	0.50000
12	5.00000	2.82843	0.00000
13	6.00000	2.82843	0.00000
14	7.00000	2.82843	0.00000
15	6.50000	3.53553	0.50000
16	7.50000	3.53553	0.50000
17	8.50000	3.53553	0.50000
18	8.00000	4.24264	0.00000
19	9.00000	4.24264	0.00000
20	10.00000	4.24264	0.00000
21	9.50000	4.94975	0.50000
22	0.61746	1.15318	0.00000
23	0.31258	1.96377	0.50000
24	1.17844	1.98101	0.00000
25	1.73941	2.80885	0.00000
26	2.04429	1.99826	0.50000
27	2.60527	2.82609	0.50000
28	3.16624	3.65393	0.50000
29	3.47112	2.84334	0.00000
30	4.03210	3.67117	0.00000
31	4.59307	4.49900	0.00000
32	4.89795	3.68842	0.50000
33	5.45892	4.51625	0.50000
34	6.01990	5.34408	0.50000
35	6.32478	4.53350	0.00000
36	6.88575	5.36133	0.00000
37	7.19063	4.55074	0.50000
38	7.75161	5.37858	0.50000
39	8.31258	6.20641	0.50000
40	8.61746	5.39582	0.00000
41	9.17844	6.22366	0.00000

[110] $\Sigma 41c$ 124.12° $(3\bar{3}8)$ $\Delta Z = 0.0$

$V^{EX} = 0.46822$

Not the densest

Contacts: 12-32, 12-32', 18-37, 18'-37

Interstitials	x	y	z	d	Touching
A	5.71132	3.74123	0.0	0.91243	15,15',32,32',33,33'
B	3.5	2.04160	0.5	0.89063	7,7',8,8',29,29'
C	2.0	1.25663	0.0	0.79106	4,4',5,5',26,26'
D	4.19637	2.95586	0.5	0.77612	10,29,29',30,30'
E	8.5	4.71682	0.0	0.70285	18,18',19,19',40,40'
F	2.90573	2.23751	0.0	0.65735	7,27,27',29
G	7.0	3.93791	0.0	0.62715	15,15',16,16',37,37'
H	5.5	3.17846	0.5	0.57800	12,12',13,13',32
I	1.15201	1.39493	0.5	0.54167	4,33,33',34,34'
J	7.61895	4.86449	0.0	0.45862	18,37,37',38,38'
K	6.04478	4.09523	0.5	0.44290	15,33,35,35'
L	2.48219	1.42683	0.5	0.43984	5,7,7',26

Substitutionals		x	y	z	d	Touching
A	29	3.5	2.39146	0.0	1.19547	7,8,29',29"
B	7	3.00351	1.85787	0.0	1.18158	8,26,26',29
C	26	2.05100	1.66189	0.5	1.11015	5,24,24',26',26"
D	10	4.23045	2.31192	0.5	1.10617	8,8',10',10",12,12',29,29'
E	4	1.53042	1.09089	0.5	1.08555	5,22,22',26
F	40	8.62155	5.19072	0.0	1.04165	19,38,38',40',40"
G	15	6.34298	3.64657	0.5	1.03665	13,13',15',15",35,35'
H	35	6.32753	4.39538	0.0	1.01900	15,15',33,33',35',35",37,37'

5.5 SUMMARY TABLE

Arranged for each section in order of increasing Σ

LEGEND

Σ	coincidence relation
Plane	boundary plane Miller indices
Angle	rotation angle of the crystals (see Section 3.3 for convention)
v^{EX}	excess volume (see Section 2.3 for definition)
L	length of the shortest repeat vector in the boundary in the plane perpendicular to the tilt axis (see Figs. 1a and 1b)
Δz	relative displacement of the two crystals in the direction of the tilt axis
INTERST.	diameter of the three largest interstitial spheres
SUBST.	diameter of the three largest substitutional spheres
SYM	symmetry elements (see Section 4.1)
	F: faceting
	G: glide-reflection
	R: screw axis rotation
	S: staggering
	CSL: exact coincidence site arrangement
A	Area of the boundary repeat unit (see Fig. 1)

[100] Σ	PLANE	ANGLE	v^{EX}	L	$\lvert\Delta Z\rvert$	INTERST.	SUBST.	SYM	A	PAGE
						0.5673	---			
5	021	53.13	0.32210	$\sqrt{10}$	0.32562	0.5326	---	S	2.2361	52
						0.5307	---			
						0.6643	---			
5	031	36.87	0.31945	$\sqrt{5}$	0.19285	0.4518	---	R	3.1623	46
						---	---			
						0.7396	---			
13a	032	67.38	0.40132	$\sqrt{26}$	-0.04929	0.6749	---	S	3.6056	62
						0.6473	---			
						0.7889	1.0564			
13a	051	22.62	0.41761	$\sqrt{13}$	0.25339	0.6017	---	R	5.0990	38
						0.4751	---			
						0.7544	---			
17a	053	61.93	0.40339	$\sqrt{17}$	0.22953	0.6265	---	RF	5.8310	56
						0.5035	---			
						0.7678	1.1214			
17a	041	28.07	0.3850	$\sqrt{34}$	---	0.7487	1.0736	S	4.1231	40
						0.5812	1.0017	CSL		
						0.8111	1.0618			
25a	043	73.74	0.45180	$\sqrt{50}$	---	0.7670	1.0558	S	5.0000	66
						0.6497	1.0233			
						0.8626	1.1921			
25a	071	16.26	0.4490	5	---	0.8381	1.1274	--	7.0711	34
						0.7379	1.0964	CSL		
						0.6243	1.0336			
29a	073	46.40	0.39735	$\sqrt{29}$	0.33908	0.6183	1.0123	RF	7.6158	50
						0.6034	---			
						0.6442	1.0170			
29a	052	43.60	0.39336	$\sqrt{58}$	0.33908	0.6427	1.0010	SF	5.3852	48
						0.6324	---			
						0.8566	1.1767			
37a	075	71.08	0.47063	$\sqrt{37}$	0.06209	0.7281	1.1221	R	8.6023	64
						0.6149	1.0549			
						0.8314	1.1309			
37a	061	18.92	0.45906	$\sqrt{74}$	-0.09288	0.8153	1.0649	S	6.0828	36
						0.6794	1.0510			
						0.8626	1.1289			
41a	054	77.32	0.48590	$\sqrt{82}$	---	0.8048	1.1159	S	6.4031	68
						0.7092	1.0909			
						0.8801	1.1404			
41a	091	12.68	0.48695	$\sqrt{41}$	-0.29703	0.7664	1.0780	R	9.0554	32
						0.6609	1.0697			
						0.8848	1.1455			
53b	095	58.11	0.48835	$\sqrt{53}$	0.10891	0.7761	1.0933	R	10.2956	54
						0.6821	1.0647			
						0.8584	1.1298			
53b	072	31.89	0.46567	$\sqrt{106}$	0.04373	0.8419	1.1088	S	7.2801	42
						0.7288	1.0958			
						0.7724	1.0517			
85	0,11,7	64.94	0.37085	$\sqrt{85}$	0.01133	0.7724	1.0138	RF	13.0384	58
						0.7259	1.0093			

[110] Σ	PLANE	ANGLE	v^{EX}	L	$\lvert\Delta Z\rvert$	INTERST.	SUBST.	SYM	A	PAGE
						0.60302	---			
3	$1\bar{1}2$	109.47	0.2092	$\sqrt{6}$	---	---	---	G	2.4495	96
						---	---			
			TWIN			---	---			
3	$1\bar{1}1$	70.53	0.0	$\sqrt{3}$	---	---	---	S	0.8660	86
						---	---	CSL		
						0.7678	1.1213			
9	$1\bar{1}4$	141.06	0.37415	$\sqrt{18}$	---	0.7311	1.1084	---	4.2426	104
						0.5811	1.0668	CSL		
						0.6480	---			
9	$2\bar{2}1$	38.94	0.26882	3	0.22401	---	---	R	1.5000	78
						---	---			
						0.4531	---			
11	$1\bar{1}3$	129.52	0.12596	$\sqrt{11}$	0.24322	0.4476	---	S	1.6583	102
						---	---			
						0.7672	1.0751			
11	$3\bar{3}2$	50.48	0.34118	$\sqrt{22}$	0.13690	0.5413	1.0664	R	4.6904	80
						---	---			
						0.7489	1.0983			
17b	$2\bar{2}3$	93.37	0.3042	$\sqrt{17}$	---	0.4978	1.0081	G†	4.1231	92
						0.4740	---			
						0.8176	1.1637			
17b	$3\bar{3}4$	86.63	0.3487	$\sqrt{34}$	---	0.6329	1.0787	G	5.8310	90
						0.4666	1.0509			
						0.7368	1.0548			
19a	$1\bar{1}6$	153.47	0.42619	$\sqrt{38}$	0.24496	0.6435	---	RF	6.1644	108
						0.5868	---			
						0.6016	---			
19a	$3\bar{3}1$	26.53	0.24066	$\sqrt{19}$	---	0.4894	---	S	2.1794	74
						0.4151	---			
						0.6484	1.0784			
27a	$1\bar{1}5$	148.42	0.3053	$\sqrt{27}$	---	0.6461	1.0119	S	2.5981	106
						0.5048	---	CSL		
						0.6367	1.0374			
27a	$5\bar{5}2$	31.58	0.31195	$\sqrt{54}$	---	0.6253	1.0022	GF	7.3485	76
						0.5518	1.0016			
						0.7462	1.0146			
33a	$1\bar{1}8$	159.95	0.42017	$\sqrt{66}$	0.13179	0.6781	1.0111	RF	8.1240	110
						0.6132	1.0060			
						0.7848	1.1082			
33a	$4\bar{4}1$	20.05	0.41711	$\sqrt{33}$	-0.13464	0.6126	1.1042	R	5.7446	72
						0.4902	1.0272			
						0.6344	1.0185			
33c	$2\bar{2}5$	121.01	0.30932	$\sqrt{33}$	0.12913	0.5705	1.0181	RF	5.7446	98
						0.5351	---			
						0.8625	1.1804			
33c	$5\bar{5}4$	58.89	0.39209	$\sqrt{66}$	0.07596	0.7263	1.1685	R	8.1240	84
						0.5966	1.0917			

[110] Σ	PLANE	ANGLE	v^{EX}	L	$\lvert\Delta Z\rvert$	INTERST.	SUBST.	SYM	A	PAGE
41c	$3\bar{3}8$	124.12	0.27305	$\sqrt{82}$	0.23311	0.5626 0.5537 0.5478	1.0057 1.0056 1.0015	RF	9.0554	100
41c	$4\bar{4}3$	55.88	0.37375	$\sqrt{41}$	0.09794	0.8270 0.6566 0.4980	1.1394 1.1277 1.0420	R	6.4031	82
43	$3\bar{3}5$	99.37	0.32277	$\sqrt{43}$	---	0.7825 0.6564 0.5103	1.1200 1.0145 1.0107	S	3.2787	94
43	$5\bar{5}6$	80.63	0.38819	$\sqrt{86}$	---	0.8818 0.7623 0.6485	1.2273 1.1691 1.1429	G	9.2736	88

† Glide vector not perpendicular to tilt axis

[111] Σ	PLANE	ANGLE	v^{EX}	L	$\lvert\Delta Z\rvert$	INTERST.	SUBST.	SYM	A	PAGE
						0.60302	----			
3	$1\bar{2}1$	60.00	0.2092	3	0.40825	----	----	---	2.4495	130

						0.7596	1.0457			
7	$2\bar{3}1$	38.21	0.37534	$\sqrt{21}$	-0.27365	0.7386	----	3S	3.7417	124
						0.5201	----			
						0.8338	1.1005			
13b	$3\bar{4}1$	27.80	0.44247	$\sqrt{39}$	0.19707	0.7880	1.0404	3S	5.0990	118
						0.6373	1.0401			
						0.8442	1.1449			
19b	$3\bar{5}2$	46.83	0.42918	$\sqrt{57}$	0.27217	0.8056	1.0423	3S	6.1644	126
						0.6959	1.0347			
						0.8742	1.1415			
21a	$4\bar{5}1$	21.79	0.47564	$\sqrt{7}$	-0.15191	0.8234	1.0938	---	6.4807	116
						0.6987	1.0905			
						0.8990	1.1749			
31a	$5\bar{6}1$	17.90	0.49482	$\sqrt{93}$	0.12292	0.8491	1.1410	3S	7.8740	114
						0.7459	1.1272			
						0.8790	1.1392			
37c	$4\bar{7}3$	50.57	0.44395	$\sqrt{111}$	0.23778	0.8581	1.0884	3S	8.6023	128
						0.7682	1.0814			
						0.8895	1.1087			
39a	$5\bar{7}2$	32.21	0.47914	$\sqrt{13}$	0.15188	0.8234	1.0767	---	8.8318	120
						0.7694	1.0606			
						0.7397	----			
3	110	60.00	0.4108	$\sqrt{3}$	0.40825	0.4861	----	---	4.2426	150
						----	----			
						0.7530	1.0574			
7	$4\bar{5}1$	38.21	0.41358	$\sqrt{7}$	-0.35902	0.6361	1.0563	R	6.4807	144
						0.6262	----			
						0.8260	1.1864			
13b	$5\bar{7}2$	27.80	0.48069	$\sqrt{13}$	0.05696	0.8121	1.1672	RF	8.8318	136
						0.7836	1.0897			
						0.8220	1.1700			
19b	$7\bar{8}1$	46.83	0.49963	$\sqrt{19}$	0.28232	0.7845	1.1137	R	10.6771	146
						0.6851	1.0136			
						0.8426	1.1430			
21a	$2\bar{3}1$	21.79	0.49375	$\sqrt{21}$	-0.24811	0.7708	1.1376	RF	11.2250	134
						0.7250	1.0946			
						0.8667	1.1702			
31a	$7,\bar{11},4$	17.90	0.49153	$\sqrt{31}$	-0.25974	0.8141	1.0981	RF	13.6382	132
						0.6938	1.0768			
						0.7519	1.0413			
37c	$10,\bar{11},1$	50.57	0.46030	$\sqrt{37}$	0.36079	0.7133	1.0287	RF	14.8997	148
						0.7016	1.0274			
						0.8707	1.1710			
39a	$3\bar{4}1$	32.21	0.45379	$\sqrt{39}$	-0.13546	0.7686	1.0621	RF	15.2971	140
						0.6914	1.0483			

EXTRA

Σ	PLANE	ANGLE	v^{EX}	L	$\lvert\Delta Z\rvert$	INTERST.	SUBST.	SYM.	A	PAGE
[100]										
						0.7527	1.0446			
5	021	53.13	0.3898	$\sqrt{10}$	---	0.5262	---	S	2.2361	154
						0.5033	---			
						0.6703	1.0238			
5	031	36.87	0.3411	$\sqrt{5}$	---	0.4695	---	G	3.1623	156
						0.4476	---			
						0.7531	1.0218			
13a	023	67.38	0.40287	$\sqrt{26}$	---	0.6733	1.0023	S	3.6056	158
						0.6346	---			
						0.8172	1.1175			
13a	023	67.38	0.4402	$\sqrt{26}$	---	0.6996	1.0860	S	3.6056	160
						0.5344	1.0220	CSL		
						0.8626	1.1726			
13a	051	22.62	0.4670	$\sqrt{13}$	---	0.8111	1.1685	---	5.0990	162
						0.6557	1.0742	CSL		
						0.7987	1.1147			
17a	053	61.93	0.42850	$\sqrt{17}$	0.09476	0.6307	1.0190	R	5.8310	164
						0.4999	---			
						0.8192	1.1204			
17a	053	61.93	0.4404	$\sqrt{17}$	---	0.7880	1.0690	---	5.8310	166
						0.6842	1.0551			
						0.8504	1.0879			
29a	073	46.40	0.46398	$\sqrt{29}$	0.15415	0.7117	1.0591	R	7.6158	168
						0.6007	1.0216			
						0.8720	1.1539			
29a	073	46.40	0.48540	$\sqrt{29}$	0.01699	0.8383	1.0948	---	7.6158	170
						0.7459	1.0910			
						0.9386	1.1620			
29a	073	46.40	0.5211	$\sqrt{29}$	---	0.8627	1.0899	---	7.6158	172
						0.7866	1.0897	CSL		
						0.8231	1.1041			
29a	052	43.60	0.4422	$\sqrt{58}$	---	0.8111	1.0785	S	5.3852	174
						0.6492	1.0468	CSL		
						0.8837	1.0793			
37a	075	71.08	0.51018	$\sqrt{37}$	---	0.8532	1.0789	---	8.6023	176
						0.7678	1.0748			
[110]										
						0.6335	1.0877			
9	$2\bar{2}1$	38.94	0.3246	3	---	0.6189	1.0099	---	3.0000	178
						0.5393	---			
						0.5807	---			
11	$1\bar{1}3$	129.52	0.1591	$\sqrt{11}$	---	0.4272	---	S	1.6583	180
						---	---			
						0.7802	1.1107			
11	$3\bar{3}2$	50.48	0.3551	$\sqrt{22}$	---	0.5517	1.0847	G	4.6904	182
						0.4606	1.0066			
						0.8290	1.1266			
19a	$1\bar{1}6$	153.47	0.4498	$\sqrt{38}$	---	0.8215	1.0774	---	6.1644	184
						0.6753	1.0518			

EXTRA

[110] Continued

19a	$3\bar{3}1$	26.53	0.2428	$\sqrt{19}$	---	0.6248 0.4846 0.4628	1.00032 1.00030 ---	S	2.1794	186
27a	$5\bar{5}2$	31.58	0.43619	$\sqrt{54}$	0.22009	0.8346 0.6931 0.5797	1.0768 1.0730 1.0378	R	7.3485	188
27a	$5\bar{5}2$	31.58	0.47211	$\sqrt{54}$	---	0.8547 0.8230 0.6963	1.1944 1.1714 1.1227	---	7.3485	190
33a	$1\bar{1}8$	159.95	0.42962	$\sqrt{66}$	0.02736	0.7920 0.7328 0.6005	1.1926 1.1015 1.0310	RF	8.1240	192
33a	$1\bar{1}8$	159.95	0.48125	$\sqrt{66}$	---	0.8662 0.8658 0.7450	1.1702 1.0912 1.0882	F	8.1240	194
33c	$2\bar{2}5$	121.01	0.41450	$\sqrt{33}$	---	0.8504 0.7847 0.6997	1.1670 1.1460 1.1100	---	5.7446	196
41c	$3\bar{3}8$	124.12	0.46822	$\sqrt{82}$	---	0.9124 0.8906 0.7911	1.1955 1.1816 1.1102	---	9.0554	198

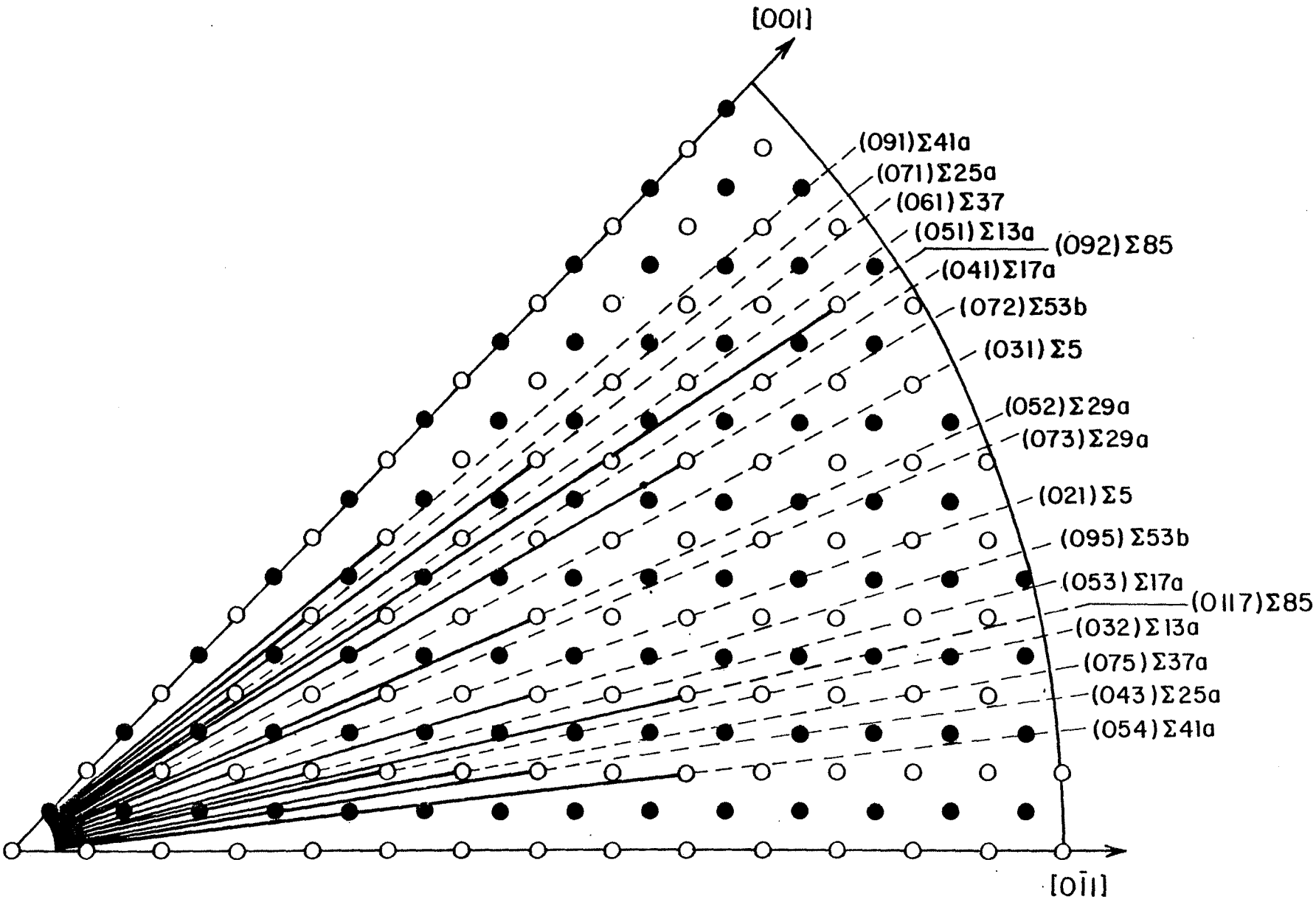


Figure 6(a) Boundary plane orientations for the [100] boundaries.

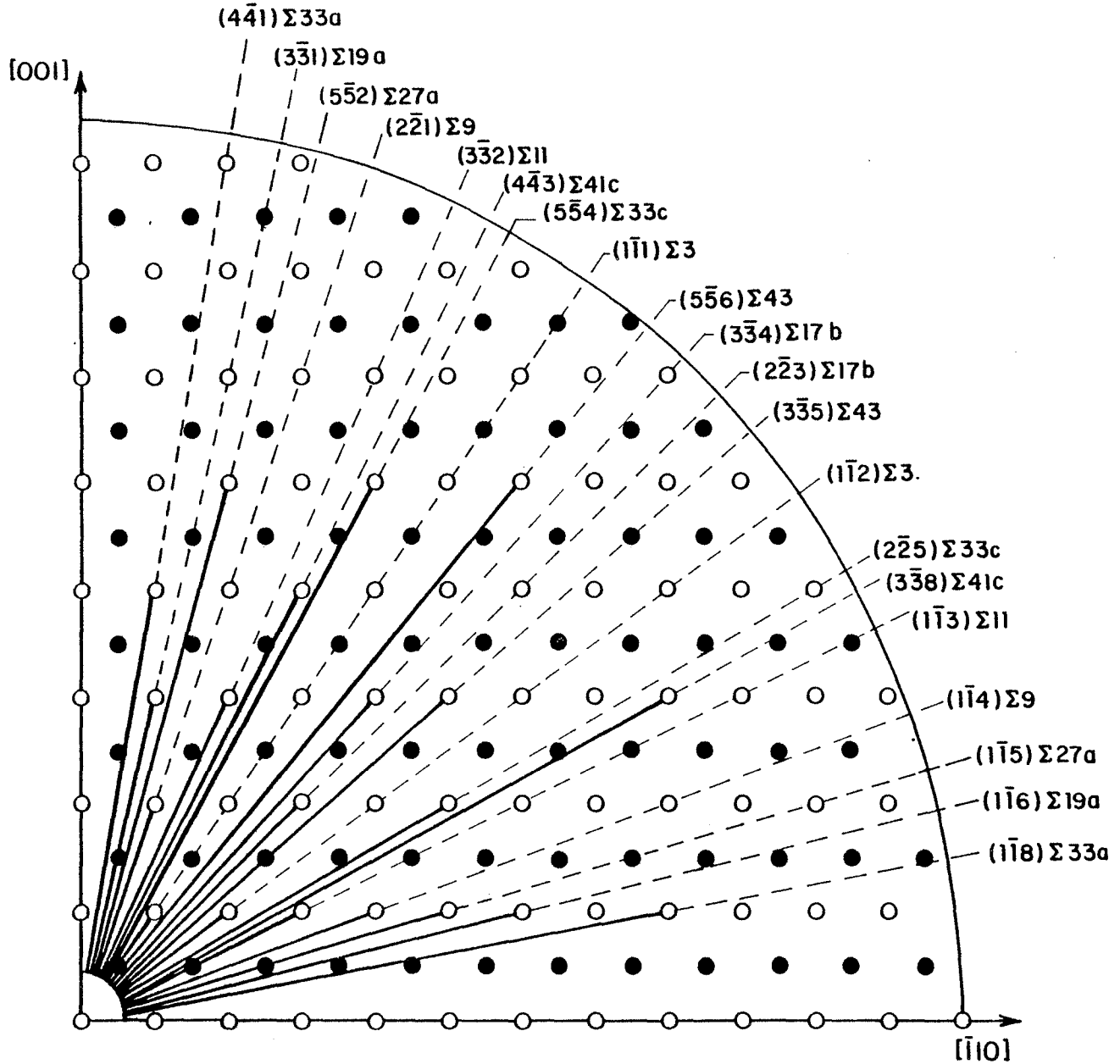


Figure 6(b) Boundary plane orientations for the [110] boundaries.

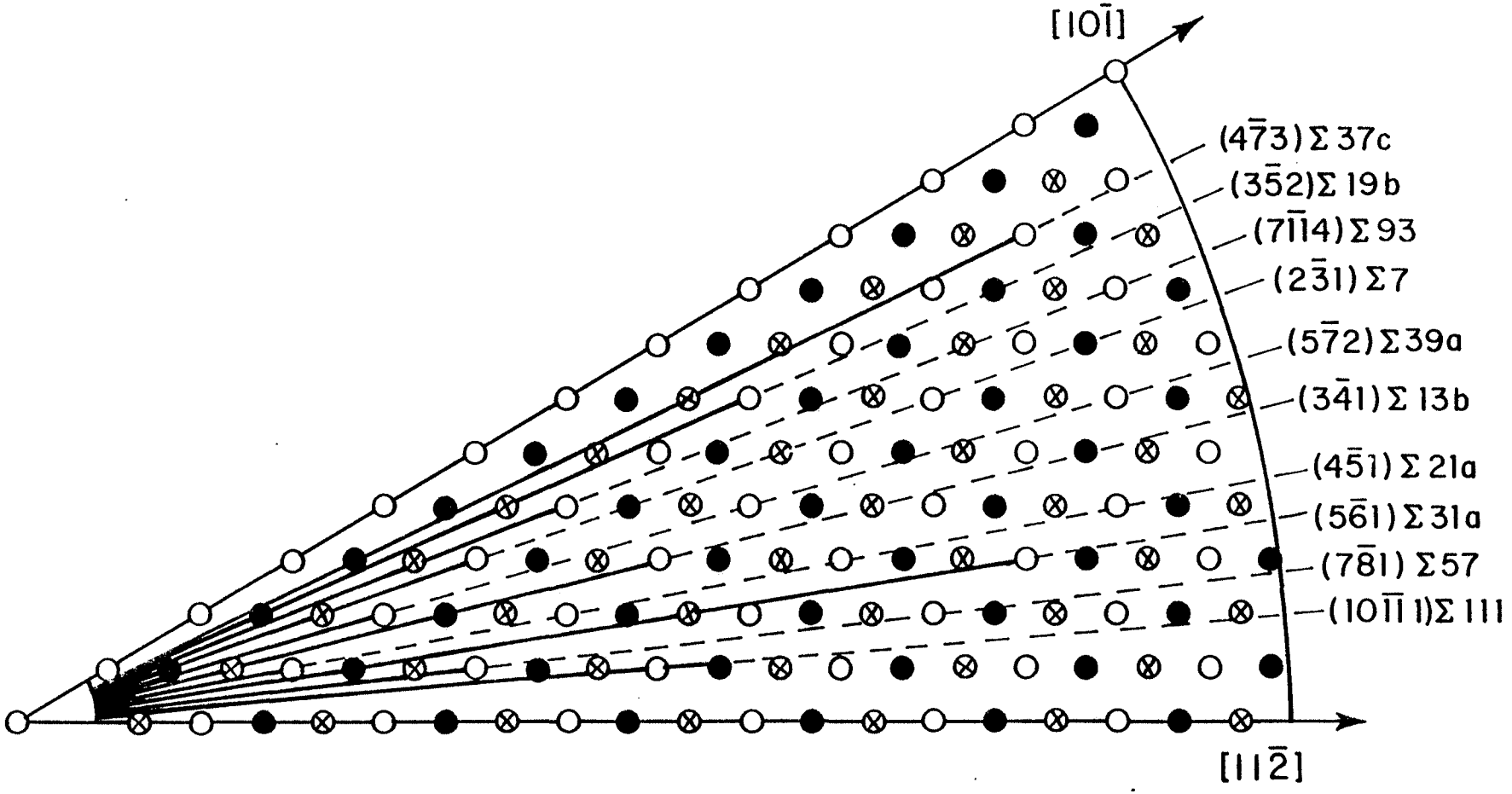


Figure 6(c) Boundary plane orientations for the [111] boundaries.

ACKNOWLEDGEMENTS

We thank Prof. M. Koiwa for pointing out the densest configurations for the $\Sigma 11$ $(1\bar{1}3)$ and $\Sigma 19b$ $(3\bar{5}2)$ boundaries, and a correction for the second densest configuration of the $\Sigma 13a$ (051) boundary.

This work has been supported by the Materials Research Laboratory at Harvard University, under Contract DMR-80-20247.

REFERENCES

1. M.F. Ashby and F. Spaepen, (1978) Scripta Met. 12, 193.

2. M.F. Ashby, F. Spaepen and S. Williams, (1978) Acta Met. 26, 1647.

3. R.C. Pond, D.A. Smith and V. Vitek, (1979) Acta Met. 27, 235.

4. H.J. Frost, M.F. Ashby and F. Spaepen (1980) Scripta Met. 14, 1051.

5. H.J. Frost, (1982) Acta Met. 30, 889.

6. D.A. Smith, V. Vitek, and R.C. Pond, (1977) Acta Met. 25, 475.

7. H.J. Frost, F. Spaepen and M.F. Ashby, (1982) Scripta Met. 16 1165.